Refinement

Refinement on F
$R = 0.030$
$wR = 0.043$
$S = 4.88$
1141 reflections
142 parameters
All H-atom parameters refined

$w = 4.62/[\sigma^2(F_o) + 0.00018F_o^2]$
$(\Delta/\sigma)_{max} = 0.01$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}
Atomic scattering factors from *SHELX*76 (Sheldrick, 1976)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	B_{eq}
C(1)	0.3036 (2)	0.3502 (2)	0.2914 (2)	1.97 (5)
C(2)	0.3155 (2)	0.5610 (2)	0.2333 (2)	1.96 (5)
C(3)	0.1632 (2)	0.6782 (2)	0.0922 (2)	2.19 (5)
C(4)	−0.0667 (2)	0.6786 (2)	0.1626 (2)	2.02 (5)
C(5)	0.3043 (2)	0.7979 (2)	0.3887 (2)	1.93 (5)
O(1)	0.3615 (2)	0.2707 (2)	0.1624 (1)	2.96 (5)
O(2)	0.2490 (2)	0.2673 (1)	0.4401 (1)	2.67 (5)
O(3)	−0.1363 (2)	0.5334 (1)	0.2339 (1)	2.59 (5)
O(4)	−0.1865 (2)	0.8513 (2)	0.1405 (2)	3.21 (5)
O(5)	0.3954 (2)	0.9005 (1)	0.2571 (1)	2.35 (5)
N(1)	0.2684 (2)	0.6299 (2)	0.3871 (2)	2.19 (5)
N(2)	0.2402 (2)	0.8508 (2)	0.5364 (2)	2.75 (5)
HO(1)	0.360 (3)	0.146 (3)	0.201 (3)	6 (1)
HO(4)	−0.315 (3)	0.841 (3)	0.184 (3)	5 (1)

Table 2. *Selected geometric parameters* (Å, °)

C(2)—C(1)	1.518 (2)	O(1)—C(1)	1.312 (2)
O(2)—C(1)	1.208 (2)	C(3)—C(2)	1.537 (2)
N(1)—C(2)	1.446 (2)	C(4)—C(3)	1.499 (2)
O(3)—C(4)	1.217 (2)	O(4)—C(4)	1.313 (2)
O(5)—C(5)	1.257 (2)	N(1)—C(5)	1.334 (2)
N(2)—C(5)	1.340 (2)		
O(1)—C(1)—C(2)	112.0 (1)	O(2)—C(1)—C(2)	123.2 (1)
O(2)—C(1)—O(1)	124.8 (1)	C(3)—C(2)—C(1)	112.1 (1)
N(1)—C(2)—C(1)	107.6 (1)	N(1)—C(2)—C(3)	111.9 (1)
C(4)—C(3)—C(2)	111.2 (1)	O(3)—C(4)—C(3)	123.5 (1)
O(4)—C(4)—C(3)	113.5 (1)	O(4)—C(4)—O(3)	123.0 (1)
N(1)—C(5)—O(5)	121.0 (1)	N(2)—C(5)—O(5)	121.9 (1)
N(2)—C(5)—N(1)	117.1 (1)	C(5)—N(1)—C(2)	123.1 (1)

Lorentz and polarization corrections were applied using the *SDP* system (Frenz, 1985). The structure was solved by direct methods using *SHELXS*86 (Sheldrick, 1985). Refinement was performed by full-matrix least-squares methods using *SHELX*76 (Sheldrick, 1976). Non-H atoms were refined anisotropically and H atoms were located in the difference maps and refined isotropically. Graphics were obtained using *ORTEP* (Johnson, 1965).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and non-bonded interactions have been deposited with the IUCr (Reference: OH1065). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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30-Dechloro-30-methoxy-25-*O*-methyl-*N*-methylnaphthomycin A

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Abstract

The reaction of naphthomycin A with methyl iodide gives the title compound as the major product.

The structure of 30-dechloro-30-methoxy-25-*O*-methyl-*N*-methylnaphthomycin A–methanol–water (1/1/1), $C_{43}H_{53}NO_{10}.CH_3OH.H_2O$, is reported and is compared with that of the minor product, the 25-*O*-methylnaphthomycin A iminomethyl ether, and with that of the analogous actamycin. Despite the chemical differences, the two naphthomycin derivatives have a very similar chair-like molecular shape, which is quite different from that of actamycin.

Comment

Naphthomycin A (1) is an antibiotic antagonist of vitamin K, active on Gram-positive bacteria and fungi. It was first obtained from cultures of *Streptomyces collinus* (strain Tu 105) (Balerna, Keller-Schierlein, Martins, Wolf & Zähner, 1969). Since then it has also been obtained by the culture of a soil sample collected in Iwo Jima, Japan, and has been shown to display significant antineoplastic activity against Ehrlich ascitic carcinoma in mice (Okabe *et al.*, 1985). The tumoricidal action seems to be due to the inhibition of various SH enzymes, especially those participating in nucleic acid biosynthesis.

The structure of naphthomycin A, a naphthalenic ansamycin, was proposed on the basis of NMR studies of the whole molecule (Williams, 1975) and of fragments obtained by chemical degradation (Brufani, Cellai & Keller-Schierlein, 1979; Cellai, Polcaro, Rossi & Brufani, 1982). In order to verify the proposed structure, and to study the correlation of structure and activity, we tried, without success, to crystallize naphthomycin A. We succeeded instead in crystallizing two derivatives of naphthomycin A, (2) and (3), obtained by methylation with CH_3I/Ag_2O (Fig. 1). The structure of naphthomycin A was thus confirmed by the X-ray analysis of the 25-*O*-methyl iminomethyl ether (2) (Keller-Schierlein *et al.*, 1984). This allowed the assignment of the absolute configuration of the chiral centres. Closely related compounds were subsequently isolated, together with naphthomycin A, from cultures of a strain (Tu 2357) of *Streptomyces aurantiogriseus* (Meyer, Keller-Schierlein, Megahed, Zähner & Segre, 1986).

The present paper reports the X-ray crystal structure of the title compound (3), the primary methylation derivative of naphthomycin A. The molecular structure of (3) is compared with that of (2) and that of the analogous actamycin 30-dechloro-2-demethyl-30-hydroxynaphthomycin A (Hambley, Parthasarathi, Rickards & Robertson, 1991).

The bond distances and valence angles in the title compound lie within normal ranges (Allen *et al.*, 1987). A perspective view of the molecular structure of (3) is shown in Fig. 2. The absolute configurations for the six

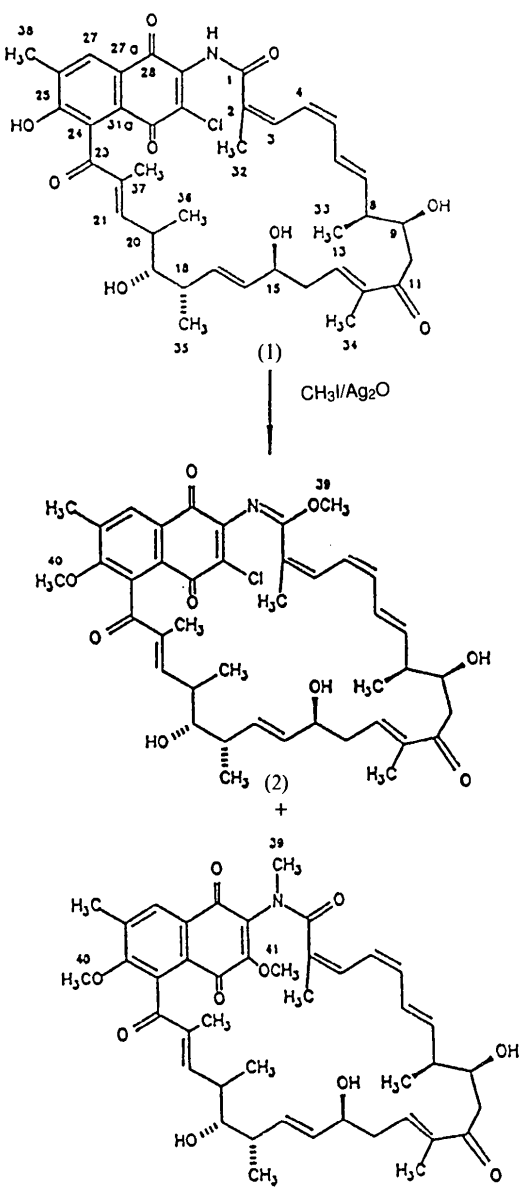

Fig. 1. Preparation of compounds (2) and (3).

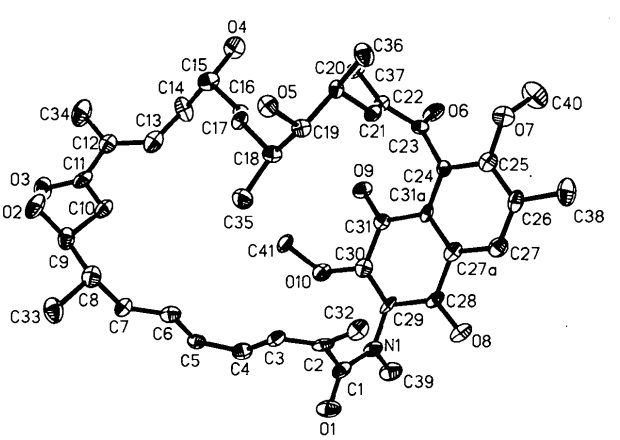

Fig. 2. A perspective view of a molecule of (3). Displacement ellipsoids are drawn at the 20% probability level.

chiral centres C8, C9, C15, C18, C19 and C20 have been assumed to be the same as in (2). The C2 and C4 double bonds have a *Z* configuration, the relevant torsion angles being −2 (1) and 1 (2)°, respectively, whereas the C6, C12, C16 and C21 double bonds have an *E* configuration, the relevant torsion angles being −176 (1), −180 (1), 177 (1) and 175 (1)°, respectively. The weighted least-squares lines through the sequences N1—C1—C2—C3 and C20—C21—C22—C23 at the junction of the ansa chain with the chromophore are almost parallel to one another, the angle between them being 10.7 (2)°.

The central part of the ansa chain from C4 to C19 takes a semicircular shape. The mean plane of this sequence makes an angle of 17.0 (1)° with that of the rings of the chromophore system. The corresponding angles are 18° for (2) and 81° for both molecules in the asymmetric unit of actamycin. As a result, (3) displays a chair-like shape (Fig. 3), very much like that observed for (2). A comparison of the conformations of (3), (2) and actamycin in terms of the skeletal torsion angles of the ansa chain connecting C24 and C29 of the naphthoquinone moiety is given in Table 2.

Despite the chemical differences between (2) and (3), they assume a very similar shape. The r.m.s. discrepancy between the dihedral angles reported in Table 2 is 4° and the best match between the two sets of corresponding atoms C1 to C31a, N1, O8 and O9 gave a weighted r.m.s. deviation of 0.28 Å.

Relevant conformational differences between the two naphthomycin derivatives and actamycin are observed at the junctions of the ansa chain with the naphthoquinone moiety along the sequences C28—C29—N1—C1—C2—C3 and C22—C23—C24—C25. As a result of the change in conformation at the C29 junction, the O atom of the amide group in actamycin is directed inwards towards the centre of the molecule, whereas in both the iminomethyl ether (2) and the *N*-methyl derivative (3) the carbonyl group is almost at a right angle to the chromophore. Furthermore, the presence of the bulky 30-chloro substituent in (2), the 30-methoxy substituent in (3) and the methyl group at C2 prevent (2) and (3) from adopting a similar conformation to that of actamycin. The less relevant difference at the C24 junction can be attributed to the presence of an intramolecular hydrogen bond between the carbonyl group at C23 and the hydroxyl group at C25 in actamycin, which is not possible in the 25-methoxy derivatives. Two other remarkable conformational differences along the sequences C12—C13—C14—C15—C16 and C17—C18—C19—C20—C21 also contribute to the quite different overall molecular shape assumed by actamycin to those of the two naphthomycin derivatives (2) and (3).

The crystal packing is shown in Fig. 4 and selected inter- and intramolecular distances are given in Table 3. Among the molecules of the reference set [the naphthomycin derivative (3), a water molecule and a molecule of methanol], hydrogen bonds link O1 to the water O atom O1*W*, and O2 to the methanol O atom O1Me. The methanol and water O atoms are also linked to the neighbouring naphthomycin molecules, resulting in infinite chains of hydrogen bonds throughout the crystal; O1*W* bridges the O atoms O7 and O1 of different naphthomycin molecules related by a twofold screw axis parallel to **a** and O1Me forms hydrogen bonds with the O atoms O2 and O4 of different naphthomycin molecules related by a twofold screw axis parallel to **b**. Each naphthomycin molecule also interacts with other molecules related by a twofold screw axis parallel to **b** by means of hydrogen bonds between O1 and O4 and between O2 and O5.

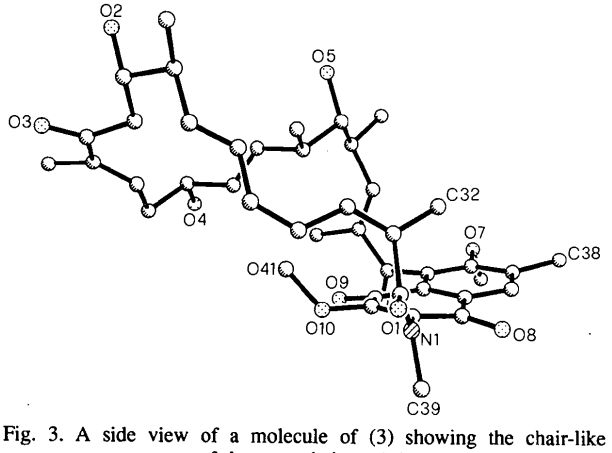

Fig. 3. A side view of a molecule of (3) showing the chair-like arrangement of the ansa chain and the chromophore.

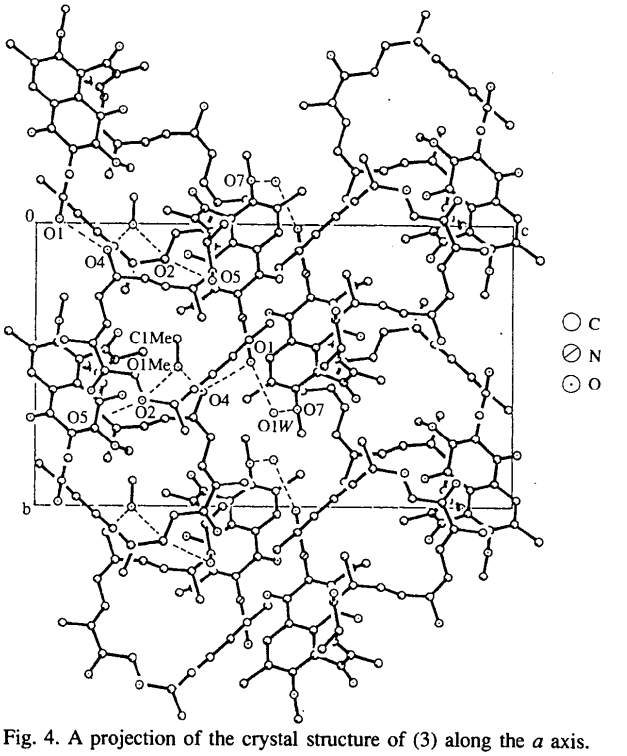

Fig. 4. A projection of the crystal structure of (3) along the *a* axis.

Experimental

The title compound (3) was prepared as described by Keller-Schierlein *et al.* (1984). Crystals suitable for data collection were grown from MeOH/H_2O at 277 K. During preliminary diffraction experiments, deterioration of the diffraction pattern due to the loss of solvent was observed. To reduce this, the crystal used for data collection was sealed in a glass capillary with the mother liquor.

Crystal data

$C_{43}H_{53}NO_{10}.CH_4O.H_2O$
M_r = 793.95
Orthorhombic
$P2_12_12_1$
a = 12.925 (3) Å
b = 14.160 (4) Å
c = 23.970 (6) Å
V = 4387 (2) Å^3
Z = 4
D_x = 1.202 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 20 reflections
θ = 25–30°
μ = 0.0812 mm^{-1}
T = 298 K
Prismatic
0.5 × 0.3 × 0.2 mm
Orange

Data collection

Four-circle diffractometer
Profile integration, ω-scan mode
Absorption correction: none
5291 measured reflections
5291 independent reflections
3002 observed reflections [$F_o > 2.0\sigma(F_o)$]
θ_{max} = 30°
$h = 0 \rightarrow 16$
$k = 0 \rightarrow 18$
$l = 0 \rightarrow 30$
3 standard reflections monitored every 97 reflections
intensity variation: ~5%

Refinement

Refinement on F
R = 0.0931
wR = 0.0828
S = 1.63
3002 reflections
514 parameters
H atoms treated using a riding model with fixed, isotropic U's
$w = 1/[\sigma^2(F) + 0.00006F^2]$
$(\Delta/\sigma)_{max}$ = 0.347
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

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

	x	y	z	U_{eq}
C1	−0.1560 (7)	0.4107 (9)	0.4443 (4)	0.062 (4)
C2	−0.0357 (7)	0.4101 (7)	0.4482 (4)	0.061 (3)
C3	0.0178 (7)	0.4674 (7)	0.4140 (4)	0.061 (3)
C4	−0.0223 (7)	0.5295 (7)	0.3716 (4)	0.064 (4)
C5	0.0354 (7)	0.5798 (7)	0.3369 (4)	0.064 (4)
C6	0.1453 (7)	0.5829 (7)	0.3332 (4)	0.060 (4)
C7	0.1991 (8)	0.6372 (7)	0.2989 (4)	0.066 (4)
C8	0.3126 (7)	0.6387 (7)	0.2912 (4)	0.068 (4)
C9	0.3431 (7)	0.6229 (7)	0.2302 (4)	0.071 (4)
C10	0.2977 (7)	0.5324 (7)	0.2083 (3)	0.064 (4)
C11	0.3043 (6)	0.5191 (9)	0.1453 (4)	0.067 (4)
C12	0.2922 (7)	0.4245 (9)	0.1202 (4)	0.067 (4)
C13	0.2511 (8)	0.3550 (9)	0.1493 (4)	0.075 (5)
C14	0.2322 (8)	0.2558 (8)	0.1321 (4)	0.085 (4)
C15	0.2937 (8)	0.1861 (8)	0.1688 (3)	0.071 (4)
C16	0.2583 (6)	0.1904 (6)	0.2286 (3)	0.053 (3)
C17	0.3098 (6)	0.2180 (6)	0.2716 (3)	0.049 (3)
C18	0.2726 (6)	0.2255 (6)	0.3306 (3)	0.053 (3)
C19	0.3357 (6)	0.1657 (6)	0.3704 (3)	0.047 (3)
C20	0.3258 (5)	0.0618 (5)	0.3587 (3)	0.042 (3)
C21	0.2199 (6)	0.0269 (6)	0.3679 (3)	0.050 (3)
C22	0.1565 (6)	−0.0188 (6)	0.3337 (3)	0.048 (3)
C23	0.0549 (6)	−0.0541 (6)	0.3535 (3)	0.051 (3)
C24	0.0123 (6)	−0.0198 (6)	0.4088 (3)	0.048 (3)
C25	0.0215 (7)	−0.0780 (8)	0.4545 (4)	0.059 (3)
C26	−0.0231 (8)	−0.0553 (8)	0.5055 (4)	0.070 (4)
C27	−0.0843 (8)	0.0271 (7)	0.5087 (3)	0.070 (4)
C27a	−0.0957 (7)	0.0865 (7)	0.4631 (3)	0.057 (3)
C28	−0.1585 (6)	0.1744 (7)	0.4687 (4)	0.055 (3)
C29	−0.1531 (6)	0.2440 (7)	0.4234 (3)	0.050 (3)
C30	−0.1035 (6)	0.2252 (7)	0.3756 (4)	0.053 (3)
C31	−0.0568 (6)	0.1303 (6)	0.3655 (3)	0.048 (3)
C31a	−0.0438 (6)	0.0637 (6)	0.4131 (3)	0.047 (3)
C32	0.0148 (7)	0.3498 (7)	0.4911 (4)	0.074 (4)
C33	0.3582 (8)	0.7316 (7)	0.3140 (4)	0.092 (5)
C34	0.3261 (10)	0.4136 (8)	0.0600 (4)	0.106 (6)
C35	0.2706 (8)	0.3296 (7)	0.3486 (4)	0.075 (4)
C36	0.3993 (8)	0.0003 (6)	0.3937 (4)	0.077 (4)
C37	0.1824 (7)	−0.0457 (7)	0.2746 (3)	0.064 (3)
C38	−0.0057 (10)	−0.1181 (8)	0.5566 (4)	0.110 (6)
C39	−0.3189 (7)	0.3302 (8)	0.4313 (5)	0.094 (5)
C40	0.0406 (9)	−0.2401 (9)	0.4414 (5)	0.108 (5)
C41	−0.0080 (7)	0.3055 (7)	0.3042 (3)	0.069 (4)
N1	−0.2034 (5)	0.3305 (6)	0.4336 (3)	0.062 (3)
O1	−0.2039 (5)	0.4854 (5)	0.4513 (3)	0.089 (3)
O2	0.4527 (5)	0.6248 (5)	0.2237 (3)	0.084 (3)
O3	0.3216 (6)	0.5893 (5)	0.1166 (3)	0.091 (3)
O4	0.2852 (6)	0.0919 (5)	0.1493 (3)	0.084 (3)
O5	0.4422 (4)	0.1965 (4)	0.3700 (2)	0.056 (2)
O6	0.0065 (5)	−0.1130 (5)	0.3278 (2)	0.073 (3)
O7	0.0852 (5)	−0.1542 (5)	0.4509 (3)	0.074 (3)
O8	−0.2082 (5)	0.1882 (5)	0.5104 (3)	0.083 (3)
O9	−0.0310 (5)	0.1062 (5)	0.3185 (2)	0.067 (2)
O10	−0.1041 (4)	0.2881 (4)	0.3331 (2)	0.063 (2)
C1Me	0.5483 (11)	0.4075 (9)	0.2963 (7)	0.129 (6)
O1Me	0.5509 (6)	0.5040 (6)	0.2982 (3)	0.108 (3)
O1*W*	−0.2014 (9)	0.6672 (7)	0.5002 (5)	0.189 (6)

Table 2. *Selected torsion angles* (°) *for the ansa chain of* (3), (2) *and actamycin*

			Actamycin[c]	
	(3)[a]	(2)[b]	molecule *A*	molecule *B*
C28—C29—N1—C1	−106 (1)	106 (1)	163 (2)	147.0 (4)
C29—N1—C1—C2	−2 (1)	−2 (1)	−178.7 (5)	165.2 (4)
N1—C1—C2—C3	122 (1)	121 (2)	−163.9 (5)	−148.9 (5)
C1—C2—C3—C4	−2 (1)	−2 (1)	6.4 (9)	3.3 (9)
C2—C3—C4—C5	−176 (1)	−172 (1)	−169.9 (6)	−166.8 (6)
C3—C4—C5—C6	1 (2)	1 (2)	10.4 (9)	4.2 (9)
C4—C5—C6—C7	−177 (1)	−179 (1)	166.6 (5)	171.0 (6)
C5—C6—C7—C8	−176 (1)	178.4 (9)	−163.6 (5)	−175.7 (5)
C6—C7—C8—C9	124 (1)	125 (1)	100.2 (6)	118.1 (6)
C7—C8—C9—C10	−56 (1)	−51 (1)	−34.8 (5)	−48.6 (7)
C8—C9—C10—C11	168 (1)	169.3 (7)	−174.2 (4)	117.4 (6)
C9—C10—C11—C12	162 (1)	164.7 (7)	−176.7 (4)	−144.5 (7)
C10—C11—C12—C13	17 (1)	12 (1)	9.7 (7)	12.8 (10)
C11—C12—C13—C14	180 (1)	177.6 (8)	179.6 (4)	179.7 (6)
C12—C13—C14—C15	118 (1)	129 (1)	170.5 (5)	−138.9 (6)
C13—C14—C15—C16	64 (1)	66 (1)	−175.1 (4)	176.7 (4)
C14—C15—C16—C17	−115 (1)	−116 (1)	−127.1 (5)	−131.4 (5)
C15—C16—C17—C18	177 (1)	177.7 (9)	176.9 (4)	−176.2 (5)
C16—C17—C18—C19	121 (1)	129.5 (9)	105.2 (6)	112.0 (6)
C17—C18—C19—C20	−65 (1)	−67.6 (9)	178.4 (4)	−176.7 (4)
C18—C19—C20—C21	−65 (1)	−69.6 (8)	177.2 (4)	−178.3 (4)
C19—C20—C21—C22	124 (1)	122.1 (9)	106.1 (6)	97.4 (6)
C20—C21—C22—C23	175 (1)	−178.7 (8)	−178.4 (5)	−178.6 (4)
C21—C22—C23—C24	14 (1)	8 (1)	30.4 (7)	23.0 (6)
C22—C23—C24—C25	−101 (1)	−104 (1)	−141.8 (5)	−134.3 (5)

References: (*a*) this work; (*b*) Keller-Schierlein *et al.* (1984); (*c*) Hambley *et al.* (1991).

Table 3. *Hydrogen-bonding geometry* (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C38—H38*A*···O7	0.96 (2)	2.36 (1)	2.84 (1)	110 (1)
C39—H39*B*···O1	0.96 (2)	2.27 (1)	2.70 (1)	106.1 (9)
C41—H41*C*···O9	0.96 (1)	2.21 (1)	2.86 (1)	123.9 (9)
O1···O1*W*	2.829 (13)	O2···O5^{ii}		2.814 (8)
O1···O4^{i}	3.032 (10)	O4···O1Me^{iii}		2.759 (11)
O2···O1Me	2.780 (11)	O7···O1*W*^{iv}		3.002 (14)

Symmetry codes: (i) $-x, \frac{1}{2}+y, \frac{1}{2}-z$; (ii) $1-x, \frac{3}{2}+y, \frac{1}{2}-z$; (iii) $1-x, y-\frac{1}{2}, \frac{1}{2}-z$; (iv) $\frac{1}{2}+x, \frac{1}{2}-y, 1-z$.

The decay of the crystal was allowed for during data reduction by applying a correction during the scaling of the data. The structure was solved by direct methods using *SIR*92 (Burla *et al.* 1992) and refined by full-matrix least-squares methods using *SHELXTL-Plus* (Sheldrick, 1990). Attempts to locate H atoms in the difference Fourier map were only partially successful. The H atoms of the O2, O4 and O5 hydroxyl groups and those of the methanol and water solvent molecules were not included in the refinement. The final cycles of refinement were carried out with H atoms riding on the corresponding C atoms with $U_{iso} = 0.08$ Å^2. Data collection and cell refinement: Siemens *R3m/V* software. Data reduction: *SHELXTL-Plus*. Molecular graphics: *SHELXTL-Plus*. Software used to prepare material for publication: *PARST* (Nardelli, 1983) and *PARSTCIF* (Nardelli, 1993).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: NA1096). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Madurahydroxylactone

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Abstract

The data acquisition for the title compound, 3,9,11,14,15-pentahydroxy-7-methoxy-10-methyl-1,3,5,6,8,13-hexahydronaphthaceno[1,2-*f*]isobenzofuran-1,8,13-trione acetonitrile solvate, $C_{26}H_{18}O_{10}.C_2H_3N$, was carried out using an image-plate detector [$T = 293$ K, $R = 0.149$, $wR = 0.120$ for 4211 unique image-plate data with $|F| > 1\sigma(F)$] and also using a scintillation detector [$T = 193$ K, $R = 0.132$, $wR = 0.121$ for 1910 unique data $> 1\sigma(F)$]. It was not possible to solve the phase problem with the scintillation detector data set, the average I/σ being too small. The structure analysis corrects the molecular structure of madurahydroxylactone suggested ambiguously by spectroscopic methods. Three of the five hydroxy groups are involved in intramolecular hydrogen bonding.

Comment

Madurahydroxylactone and homologues were isolated from the culture broth of *Actinomadura rubra* by extraction, precipitation and high-performance liquid chromatography (HPLC) methods (Fleck, Strauss, Meyer & Porstendorfer, 1978). Four compounds were initially found which differed only by the type of alkoxy group at the hydroxylactone function of the natural basic molecule. These compounds were identified as methoxy, ethoxy, propoxy and butoxy derivatives of 'maduranic acid' (Strauss & Fleck, 1990; Strauss *et al.*, 1990) and they have strong antimicrobial activity against Gram-positive bacteria. Two possible structures were suggested from spectroscopic methods (Strauss & Fleck, 1990; Miosga, Römer & Hesse, 1985). Because a high degree of ambiguity remained, we decided to carry out an X-ray structure analysis of 'maduranic acid'. Figs. 1 and 2 show the results of the structure analysis. The hydroxylactone form is obtained when the carboxyl and