Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Roridin H

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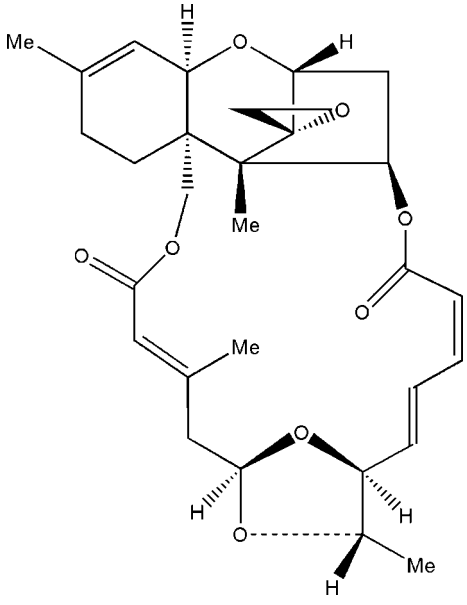
Received 15 May 2007; accepted 21 May 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.051; wR factor = 0.128; data-to-parameter ratio = 8.9.

In the molecule of the title compound, $C_{29}H_{36}O_8$, the five-membered rings adopt envelope conformations, while the six-membered rings have twist and chair conformations. The five-membered rings also have pseudo-mirror planes, while the six-membered rings have pseudo-twofold axes. In the crystal structure, intra- and intermolecular C—H···O hydrogen bonds cause the formation of a network structure. This study establishes the relative configuration of the compound.

Related literature

For general backgroud, see: Amagata *et al.* (2003); Namikoshi *et al.* (2001); Alvi *et al.* (2002); Xu *et al.* (2006); Abbas *et al.* (2002); Kaneko *et al.* (1982); Allen *et al.* (1987); Jarvis & Midiwo (1982); Cremer & Pople (1975). For related literature, see: Shen *et al.* (2006).



Experimental

Crystal data

$C_{29}H_{36}O_8$
M_r = 512.58
Monoclinic, $P2_1$
a = 10.259 (6) Å
b = 8.989 (5) Å
c = 14.290 (8) Å
β = 96.410 (7)°
V = 1309.6 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.25 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.977, T_{max} = 0.981
6524 measured reflections
3012 independent reflections
2555 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.128
S = 1.09
3012 reflections
338 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C30—H30B···O2	0.96	2.36	2.864 (4)	112
C30—H30B···O29	0.96	2.64	3.322 (5)	129
C12—H12···O29	0.93	2.33	2.940 (4)	123
C26—H26C···O25	0.96	2.24	2.989 (5)	134
C1—H1B···O20^{i}	0.97	2.52	3.430 (4)	157
C2′—H2′A···O29^{ii}	0.97	2.63	3.252 (5)	122

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

This study was supported by the National Natural Science Foundation of China (grant No. 30371680). We thank Professor Min-Qin Chen of the Research Centre of Analysis and Measurement of Fudan University for work on the X-ray crystal structure determination.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2249).

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  doi:10.1107/S1600536807024786

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supplementary materials

Acta Cryst. (2007). E**63**, o2990-o2991 [**doi:10.1107/S1600536807024786**]

Roridin H

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Comment

Macrocyclic trichothecenes have attracted considerable interest mainly due to their potent biological activity, such as cancer prevention (Amagata *et al.*, 2003), cytotoxicity (Namikoshi *et al.*, 2001; Alvi *et al.*, 2002; Xu *et al.*, 2006) and phytotoxicity (Abbas *et al.*, 2002). Knowledge of the three-dimensional structure of these compounds is important in order to establish structure-activity relationships (Kaneko *et al.*, 1982). We herein report the crystal structure of roridin H, (I), a bioactive macrocyclic trichothecene with systematic name Spiro[7,10-epoxy-17,19-methano-1H,3*H*,9H,24*H*-[1,6,12]trioxacyclo- nonadecino[3,\4 − d][1]benzopyran-18(19*H*),2'-oxirane], verrucarin A derivative.

In the molecule of the title compound, (I), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987; Jarvis & Midiwo, 1982). Rings A (O8/O27/C7/C9/C10) and B (C1'/C17A/C17—C19) have envelope conformations with atoms C9 and C18 displaced by −0.556 (3) Å and −0.671 (3) Å from the planes of the other four ring atoms, respectively. Rings C (C20A/C24A/C21—C24) and D (O20/C17A/C18/C19/C20A/C24A) are not planar, having total puckering amplitudes, Q_T, of 0.464 (3) and 0.637 (3) Å, respectively and twist and chair conformations φ = 91.55 (6)°, θ = 131.26 (4)° and φ = 66.76 (3)°, θ = 161.87 (3)° (Cremer & Pople, 1975). The five-membered rings A and B have pseudo mirror planes running through C9 and the mid-point of C7—O27 bond (for ring A) and C18 and the mid-point of C1'-C17 bond (for ring B), while the six-membered rings C and D have pseudo twofold axes passing through the mid-points of C18—C19 and C20A—C24A bonds (for ring C) and C21—C22 and C24—C24A bonds (for ring D), as can be deduced from the torsion angles (Table 1).

There is no significant anomalous dispersion for the determination of the absolute configuration. However, the relative configuration for the molecule was definitely determined and the absolute configurations in the trichothecene moiety were certain (Shen *et al.*, 2006), thus C17*R*, C17aS, C18S, C19*R*, C20aR, C24aR were presumed in (I) and the absolute configurations of C9S and C10S would be deduced. This absolute configuration of the molecule needs to be verified.

In the crystal structure, the weak intra- and intermolecular C—H···O hydrogen bonds (Table 2) cause to the formation of a network structure (Fig. 2), in which they may be effective in the stabilization of the structure.

Experimental

The title compound, (I), was isolated from 3*L* culture of the fungal strain S_{1-1} (a *Myrothecium sp.*), affording 3.2 mg by repeated column chromatography on Sephadex LH-20 and Silica gel. *Pyricularia oryzae* was grown on a slant culture medium consisting of yeast extract 0.2%, soluble starch 1% and agar 2% at 300 K for 12~14 days, using as the indicator organism of the antifungal activity. Single crystals suitable for X-ray analysis were obtained from acetone by slow evaporation at room temperature.

Refinement

Friedel pairs were merged before the final refinement, as there is no significant anomalous dispersion for the determination of the absolute configuration. H atoms were positioned geometrically, with C—H = 0.93, 0.98, 0.97 and 0.96 Å for aromatic, methine, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.5 for methyl H and x = 1.2 for all other H atoms.

Figures

Fig. 1. The molecular structure of (I) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

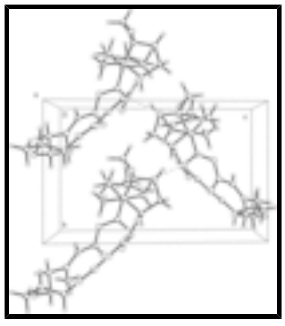

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

(I)

Crystal data

$C_{29}H_{36}O_8$	F_{000} = 548
M_r = 512.58	D_x = 1.300 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 940 reflections
a = 10.259 (6) Å	θ = 2.6–23.2º
b = 8.989 (5) Å	μ = 0.09 mm^{-1}
c = 14.290 (8) Å	T = 293 (2) K
β = 96.410 (7)º	Prism, colorless
V = 1309.6 (13) Å^3	0.25 × 0.20 × 0.20 mm
Z = 2	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3012 independent reflections
Radiation source: fine-focus sealed tube	2555 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.044

T = 293(2) K	θ_{max} = 27.0º
φ and ω scans	θ_{min} = 1.4º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −13→13
T_{min} = 0.977, T_{max} = 0.981	k = −10→11
6524 measured reflections	l = −12→18

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.051	$w = 1/[\sigma^2(F_o^2) + (0.0693P)^2 + 0.0186P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.128	$(\Delta/\sigma)_{max} < 0.001$
S = 1.09	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
3012 reflections	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
338 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), with no Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0 (10)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5453 (3)	0.3762 (3)	0.6923 (2)	0.0384 (6)
H1A	0.6405	0.3773	0.7013	0.046*
H1B	0.5165	0.4447	0.6418	0.046*
O2	0.4955 (2)	0.4239 (2)	0.77738 (14)	0.0419 (5)
C3	0.5125 (3)	0.5676 (4)	0.7996 (2)	0.0483 (7)
C4	0.4303 (4)	0.6080 (4)	0.8736 (2)	0.0500 (8)
H4	0.3609	0.5443	0.8814	0.060*
C5	0.4437 (4)	0.7245 (4)	0.9306 (2)	0.0502 (8)
C6	0.3512 (4)	0.7469 (4)	1.0042 (2)	0.0572 (9)

H6A	0.4028	0.7610	1.0647	0.069*
H6B	0.3003	0.6566	1.0083	0.069*
C7	0.2570 (4)	0.8766 (5)	0.9873 (3)	0.0602 (9)
H7	0.3071	0.9697	0.9901	0.072*
O8	0.1679 (3)	0.8806 (4)	1.05537 (18)	0.0714 (8)
C9	0.0537 (4)	0.8063 (5)	1.0137 (3)	0.0647 (10)
H9	0.0685	0.6986	1.0171	0.078*
C10	0.0486 (4)	0.8563 (5)	0.9119 (3)	0.0619 (10)
H10	0.0105	0.9563	0.9061	0.074*
C11	−0.0257 (4)	0.7571 (5)	0.8415 (3)	0.0616 (10)
H11	−0.1158	0.7491	0.8433	0.074*
C12	0.0264 (4)	0.6798 (4)	0.7767 (2)	0.0539 (8)
H12	0.1159	0.6887	0.7727	0.065*
C13	−0.0495 (3)	0.5820 (5)	0.7119 (2)	0.0564 (9)
H13	−0.1394	0.5805	0.7153	0.068*
C14	−0.0053 (3)	0.4928 (5)	0.6470 (2)	0.0537 (8)
H14	−0.0666	0.4379	0.6085	0.064*
C15	0.1339 (3)	0.4763 (4)	0.6332 (2)	0.0448 (7)
O16	0.1512 (2)	0.3506 (3)	0.58600 (15)	0.0472 (5)
C17	0.2858 (3)	0.3108 (4)	0.5746 (2)	0.0391 (6)
H17	0.3405	0.3999	0.5726	0.047*
C17A	0.3426 (3)	0.2037 (3)	0.6553 (2)	0.0354 (6)
C18	0.3089 (3)	0.0526 (4)	0.6096 (2)	0.0411 (7)
C19	0.3448 (3)	0.0706 (4)	0.5121 (2)	0.0431 (7)
H19	0.3056	−0.0084	0.4709	0.052*
O20	0.4846 (2)	0.0672 (2)	0.51674 (14)	0.0411 (5)
C20A	0.5468 (3)	0.1918 (3)	0.5675 (2)	0.0349 (6)
H20A	0.5295	0.2816	0.5292	0.042*
C21	0.6912 (3)	0.1586 (4)	0.5744 (2)	0.0445 (7)
H21	0.7318	0.1665	0.5196	0.053*
C22	0.7645 (3)	0.1194 (4)	0.6515 (3)	0.0499 (8)
C23	0.7103 (3)	0.1063 (5)	0.7434 (2)	0.0562 (9)
H23A	0.7409	0.1900	0.7828	0.067*
H23B	0.7443	0.0163	0.7747	0.067*
C24	0.5609 (3)	0.1021 (4)	0.7350 (2)	0.0427 (7)
H24A	0.5324	0.1199	0.7965	0.051*
H24B	0.5311	0.0037	0.7145	0.051*
C24A	0.4972 (3)	0.2185 (3)	0.66494 (18)	0.0331 (6)
O25	0.5840 (4)	0.6482 (3)	0.7619 (2)	0.0807 (10)
C26	0.5507 (5)	0.8364 (6)	0.9300 (3)	0.0880 (16)
H26A	0.6065	0.8317	0.9885	0.132*
H26B	0.5132	0.9341	0.9222	0.132*
H26C	0.6012	0.8155	0.8789	0.132*
O27	0.1828 (3)	0.8649 (4)	0.89813 (17)	0.0668 (7)
C28	−0.0622 (5)	0.8447 (7)	1.0651 (3)	0.0907 (16)
H28A	−0.0418	0.8231	1.1309	0.136*
H28B	−0.1367	0.7868	1.0401	0.136*
H28C	−0.0821	0.9485	1.0571	0.136*
O29	0.2216 (3)	0.5599 (3)	0.66110 (19)	0.0610 (7)

C30	0.2802 (3)	0.2202 (4)	0.7473 (2)	0.0437 (7)
H30A	0.1910	0.1864	0.7380	0.066*
H30B	0.2822	0.3229	0.7659	0.066*
H30C	0.3284	0.1618	0.7956	0.066*
O31	0.1813 (2)	−0.0075 (3)	0.6160 (2)	0.0624 (7)
C32	0.9084 (3)	0.0833 (6)	0.6520 (3)	0.0743 (12)
H32A	0.9217	−0.0214	0.6621	0.111*
H32B	0.9582	0.1377	0.7016	0.111*
H32C	0.9368	0.1108	0.5926	0.111*
C1'	0.2847 (3)	0.2206 (4)	0.4835 (2)	0.0504 (8)
H1'A	0.1957	0.2083	0.4537	0.061*
H1'B	0.3359	0.2704	0.4397	0.061*
C2'	0.2946 (4)	−0.0883 (4)	0.6567 (3)	0.0586 (9)
H2'A	0.3185	−0.1781	0.6250	0.070*
H2'B	0.3121	−0.0906	0.7248	0.070*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0381 (15)	0.0391 (15)	0.0392 (14)	−0.0056 (12)	0.0091 (12)	−0.0044 (12)
O2	0.0493 (12)	0.0388 (11)	0.0389 (11)	−0.0044 (9)	0.0111 (9)	−0.0051 (9)
C3	0.059 (2)	0.0400 (17)	0.0468 (17)	−0.0055 (16)	0.0098 (14)	−0.0033 (14)
C4	0.063 (2)	0.0423 (18)	0.0467 (17)	−0.0073 (15)	0.0149 (15)	−0.0019 (14)
C5	0.069 (2)	0.0438 (18)	0.0380 (15)	0.0022 (16)	0.0067 (15)	−0.0003 (14)
C6	0.085 (3)	0.050 (2)	0.0377 (16)	0.0062 (18)	0.0119 (16)	−0.0040 (14)
C7	0.081 (3)	0.049 (2)	0.0531 (19)	0.0025 (19)	0.0179 (18)	−0.0097 (17)
O8	0.087 (2)	0.0735 (19)	0.0569 (14)	0.0052 (16)	0.0204 (14)	−0.0208 (14)
C9	0.086 (3)	0.054 (2)	0.058 (2)	0.006 (2)	0.025 (2)	−0.0090 (18)
C10	0.077 (3)	0.051 (2)	0.060 (2)	0.0157 (19)	0.0180 (19)	−0.0035 (18)
C11	0.065 (2)	0.061 (2)	0.059 (2)	0.0185 (19)	0.0129 (18)	−0.0032 (18)
C12	0.057 (2)	0.057 (2)	0.0486 (18)	0.0120 (17)	0.0098 (15)	0.0035 (15)
C13	0.0445 (18)	0.070 (2)	0.0542 (19)	0.0191 (17)	0.0031 (15)	−0.0016 (18)
C14	0.0450 (18)	0.056 (2)	0.0578 (19)	0.0118 (16)	−0.0030 (15)	−0.0070 (17)
C15	0.0484 (18)	0.0376 (16)	0.0489 (17)	0.0076 (14)	0.0074 (14)	−0.0005 (14)
O16	0.0343 (11)	0.0468 (13)	0.0600 (13)	0.0067 (9)	0.0024 (9)	−0.0108 (11)
C17	0.0328 (14)	0.0404 (16)	0.0443 (15)	0.0054 (12)	0.0054 (12)	−0.0030 (12)
C17A	0.0301 (14)	0.0363 (16)	0.0411 (14)	−0.0011 (11)	0.0105 (11)	−0.0040 (12)
C18	0.0296 (14)	0.0370 (16)	0.0575 (17)	−0.0040 (12)	0.0084 (12)	−0.0109 (13)
C19	0.0379 (15)	0.0452 (17)	0.0458 (16)	0.0007 (13)	0.0022 (12)	−0.0164 (14)
O20	0.0369 (11)	0.0402 (12)	0.0475 (11)	0.0019 (9)	0.0097 (8)	−0.0121 (10)
C20A	0.0335 (14)	0.0331 (14)	0.0393 (14)	−0.0013 (11)	0.0099 (11)	−0.0043 (11)
C21	0.0379 (16)	0.0455 (18)	0.0536 (18)	−0.0036 (13)	0.0203 (14)	−0.0064 (14)
C22	0.0326 (15)	0.0478 (19)	0.070 (2)	−0.0011 (14)	0.0100 (15)	−0.0031 (16)
C23	0.0418 (17)	0.065 (2)	0.060 (2)	0.0035 (16)	−0.0034 (15)	0.0081 (18)
C24	0.0410 (16)	0.0460 (18)	0.0418 (15)	−0.0005 (13)	0.0080 (12)	0.0057 (13)
C24A	0.0326 (13)	0.0334 (15)	0.0344 (13)	−0.0013 (11)	0.0085 (11)	−0.0009 (11)
O25	0.112 (2)	0.0499 (16)	0.090 (2)	−0.0335 (16)	0.0539 (19)	−0.0207 (14)
C26	0.117 (4)	0.074 (3)	0.078 (3)	−0.032 (3)	0.032 (3)	−0.033 (2)

O27	0.0792 (18)	0.0735 (18)	0.0496 (13)	−0.0002 (15)	0.0160 (12)	0.0037 (13)
C28	0.098 (3)	0.103 (4)	0.078 (3)	0.009 (3)	0.037 (3)	−0.019 (3)
O29	0.0579 (15)	0.0452 (14)	0.0838 (17)	−0.0043 (12)	0.0257 (13)	−0.0147 (13)
C30	0.0364 (15)	0.0485 (18)	0.0487 (17)	−0.0028 (13)	0.0164 (13)	−0.0059 (14)
O31	0.0411 (13)	0.0580 (15)	0.0908 (18)	−0.0157 (12)	0.0191 (12)	−0.0186 (14)
C32	0.0348 (18)	0.089 (3)	0.100 (3)	0.010 (2)	0.0119 (19)	0.005 (3)
C1'	0.0440 (17)	0.059 (2)	0.0469 (17)	0.0107 (16)	0.0000 (13)	−0.0079 (15)
C2'	0.056 (2)	0.043 (2)	0.079 (3)	−0.0100 (16)	0.0181 (18)	−0.0061 (18)

Geometric parameters (Å, °)

C1—O2	1.436 (3)	C17A—C30	1.532 (4)
C1—C24A	1.538 (4)	C17A—C24A	1.582 (4)
C1—H1A	0.9700	C18—O31	1.428 (4)
C1—H1B	0.9700	C18—C2'	1.449 (5)
O2—C3	1.337 (4)	C18—C19	1.489 (4)
C3—O25	1.201 (4)	C19—O20	1.428 (4)
C3—C4	1.470 (5)	C19—C1'	1.520 (5)
C4—C5	1.324 (5)	C19—H19	0.9800
C4—H4	0.9300	O20—C20A	1.444 (3)
C5—C26	1.489 (6)	C20A—C21	1.504 (4)
C5—C6	1.507 (5)	C20A—C24A	1.553 (4)
C6—C7	1.517 (6)	C20A—H20A	0.9800
C6—H6A	0.9700	C21—C22	1.311 (5)
C6—H6B	0.9700	C21—H21	0.9300
C7—O8	1.407 (5)	C22—C23	1.487 (5)
C7—O27	1.414 (5)	C22—C32	1.511 (5)
C7—H7	0.9800	C23—C24	1.524 (5)
O8—C9	1.421 (5)	C23—H23A	0.9700
C9—C28	1.506 (6)	C23—H23B	0.9700
C9—C10	1.518 (5)	C24—C24A	1.542 (4)
C9—H9	0.9800	C24—H24A	0.9700
C10—O27	1.415 (5)	C24—H24B	0.9700
C10—C11	1.489 (6)	C26—H26A	0.9599
C10—H10	0.9800	C26—H26B	0.9599
C11—C12	1.317 (5)	C26—H26C	0.9599
C11—H11	0.9300	C28—H28A	0.9599
C12—C13	1.441 (5)	C28—H28B	0.9599
C12—H12	0.9300	C28—H28C	0.9599
C13—C14	1.341 (5)	C30—H30A	0.9599
C13—H13	0.9300	C30—H30B	0.9599
C14—C15	1.471 (5)	C30—H30C	0.9599
C14—H14	0.9300	O31—C2'	1.437 (5)
C15—O29	1.206 (4)	C32—H32A	0.9599
C15—O16	1.338 (4)	C32—H32B	0.9599
O16—C17	1.453 (3)	C32—H32C	0.9599
C17—C1'	1.533 (4)	C1'—H1'A	0.9700
C17—C17A	1.564 (4)	C1'—H1'B	0.9700
C17—H17	0.9800	C2'—H2'A	0.9700

C17A—C18	1.530 (4)	C2'—H2'B	0.9700
O2—C1—C24A	110.8 (2)	O20—C19—C18	107.8 (2)
O2—C1—H1A	109.5	O20—C19—C1'	114.0 (3)
C24A—C1—H1A	109.5	C18—C19—C1'	102.3 (3)
O2—C1—H1B	109.5	O20—C19—H19	110.8
C24A—C1—H1B	109.5	C18—C19—H19	110.8
H1A—C1—H1B	108.1	C1'—C19—H19	110.8
C3—O2—C1	116.1 (2)	C19—O20—C20A	113.1 (2)
O25—C3—O2	123.1 (3)	O20—C20A—C21	104.8 (2)
O25—C3—C4	127.0 (3)	O20—C20A—C24A	113.6 (2)
O2—C3—C4	109.8 (3)	C21—C20A—C24A	113.0 (2)
C5—C4—C3	127.5 (3)	O20—C20A—H20A	108.4
C5—C4—H4	116.2	C21—C20A—H20A	108.4
C3—C4—H4	116.2	C24A—C20A—H20A	108.4
C4—C5—C26	123.8 (3)	C22—C21—C20A	125.2 (3)
C4—C5—C6	120.3 (3)	C22—C21—H21	117.4
C26—C5—C6	115.8 (3)	C20A—C21—H21	117.4
C5—C6—C7	115.5 (3)	C21—C22—C23	121.9 (3)
C5—C6—H6A	108.4	C21—C22—C32	122.0 (3)
C7—C6—H6A	108.4	C23—C22—C32	116.1 (3)
C5—C6—H6B	108.4	C22—C23—C24	113.8 (3)
C7—C6—H6B	108.4	C22—C23—H23A	108.8
H6A—C6—H6B	107.5	C24—C23—H23A	108.8
O8—C7—O27	107.4 (3)	C22—C23—H23B	108.8
O8—C7—C6	111.1 (3)	C24—C23—H23B	108.8
O27—C7—C6	110.8 (3)	H23A—C23—H23B	107.7
O8—C7—H7	109.2	C23—C24—C24A	112.6 (3)
O27—C7—H7	109.2	C23—C24—H24A	109.1
C6—C7—H7	109.2	C24A—C24—H24A	109.1
C7—O8—C9	105.5 (3)	C23—C24—H24B	109.1
O8—C9—C28	110.3 (3)	C24A—C24—H24B	109.1
O8—C9—C10	101.6 (3)	H24A—C24—H24B	107.8
C28—C9—C10	117.0 (4)	C1—C24A—C24	111.1 (2)
O8—C9—H9	109.2	C1—C24A—C20A	104.0 (2)
C28—C9—H9	109.2	C24—C24A—C20A	108.6 (2)
C10—C9—H9	109.2	C1—C24A—C17A	113.0 (2)
O27—C10—C11	111.8 (3)	C24—C24A—C17A	110.4 (2)
O27—C10—C9	102.7 (3)	C20A—C24A—C17A	109.6 (2)
C11—C10—C9	115.5 (4)	C5—C26—H26A	109.5
O27—C10—H10	108.9	C5—C26—H26B	109.5
C11—C10—H10	108.9	H26A—C26—H26B	109.5
C9—C10—H10	108.9	C5—C26—H26C	109.5
C12—C11—C10	125.0 (4)	H26A—C26—H26C	109.5
C12—C11—H11	117.5	H26B—C26—H26C	109.5
C10—C11—H11	117.5	C7—O27—C10	108.2 (3)
C11—C12—C13	122.8 (4)	C9—C28—H28A	109.5
C11—C12—H12	118.6	C9—C28—H28B	109.5
C13—C12—H12	118.6	H28A—C28—H28B	109.5
C14—C13—C12	127.5 (3)	C9—C28—H28C	109.5

C14—C13—H13	116.2	H28A—C28—H28C	109.5
C12—C13—H13	116.2	H28B—C28—H28C	109.5
C13—C14—C15	124.1 (3)	C17A—C30—H30A	109.5
C13—C14—H14	117.9	C17A—C30—H30B	109.5
C15—C14—H14	117.9	H30A—C30—H30B	109.5
O29—C15—O16	123.8 (3)	C17A—C30—H30C	109.5
O29—C15—C14	126.4 (3)	H30A—C30—H30C	109.5
O16—C15—C14	109.8 (3)	H30B—C30—H30C	109.5
C15—O16—C17	116.5 (2)	C18—O31—C2'	60.8 (2)
O16—C17—C1'	108.0 (2)	C22—C32—H32A	109.5
O16—C17—C17A	110.4 (2)	C22—C32—H32B	109.5
C1'—C17—C17A	105.5 (3)	H32A—C32—H32B	109.5
O16—C17—H17	110.9	C22—C32—H32C	109.5
C1'—C17—H17	110.9	H32A—C32—H32C	109.5
C17A—C17—H17	110.9	H32B—C32—H32C	109.5
C18—C17A—C30	110.9 (2)	C19—C1'—C17	106.0 (3)
C18—C17A—C17	100.6 (2)	C19—C1'—H1'A	110.5
C30—C17A—C17	114.6 (2)	C17—C1'—H1'A	110.5
C18—C17A—C24A	106.7 (2)	C19—C1'—H1'B	110.5
C30—C17A—C24A	115.3 (2)	C17—C1'—H1'B	110.5
C17—C17A—C24A	107.4 (2)	H1'A—C1'—H1'B	108.7
O31—C18—C2'	59.9 (2)	O31—C2'—C18	59.3 (2)
O31—C18—C19	115.2 (3)	O31—C2'—H2'A	117.8
C2'—C18—C19	125.3 (3)	C18—C2'—H2'A	117.8
O31—C18—C17A	118.2 (2)	O31—C2'—H2'B	117.8
C2'—C18—C17A	127.4 (3)	C18—C2'—H2'B	117.8
C19—C18—C17A	103.6 (3)	H2'A—C2'—H2'B	115.0
C24A—C1—O2—C3	−169.2 (3)	O31—C18—C19—C1'	84.4 (3)
C1—O2—C3—O25	−12.7 (5)	C2'—C18—C19—C1'	154.2 (3)
C1—O2—C3—C4	166.3 (3)	C17A—C18—C19—C1'	−46.2 (3)
O25—C3—C4—C5	−20.0 (7)	C18—C19—O20—C20A	−65.4 (3)
O2—C3—C4—C5	161.0 (3)	C1'—C19—O20—C20A	47.4 (3)
C3—C4—C5—C26	−1.4 (6)	C19—O20—C20A—C21	173.5 (2)
C3—C4—C5—C6	−178.8 (4)	C19—O20—C20A—C24A	49.6 (3)
C4—C5—C6—C7	−110.5 (4)	O20—C20A—C21—C22	−108.2 (3)
C26—C5—C6—C7	72.0 (5)	C24A—C20A—C21—C22	16.0 (4)
C5—C6—C7—O8	175.1 (3)	C20A—C21—C22—C23	−1.3 (5)
C5—C6—C7—O27	55.7 (5)	C20A—C21—C22—C32	178.1 (4)
O27—C7—O8—C9	25.6 (4)	C21—C22—C23—C24	15.1 (5)
C6—C7—O8—C9	−95.7 (4)	C32—C22—C23—C24	−164.3 (4)
C7—O8—C9—C28	−161.9 (4)	C22—C23—C24—C24A	−43.9 (4)
C7—O8—C9—C10	−37.1 (4)	O2—C1—C24A—C24	−69.2 (3)
O8—C9—C10—O27	35.1 (4)	O2—C1—C24A—C20A	174.1 (2)
C28—C9—C10—O27	155.3 (4)	O2—C1—C24A—C17A	55.4 (3)
O8—C9—C10—C11	157.1 (3)	C23—C24—C24A—C1	−56.7 (3)
C28—C9—C10—C11	−82.7 (5)	C23—C24—C24A—C20A	57.1 (3)
O27—C10—C11—C12	3.3 (6)	C23—C24—C24A—C17A	177.2 (3)
C9—C10—C11—C12	−113.6 (4)	O20—C20A—C24A—C1	−164.7 (2)
C10—C11—C12—C13	178.2 (4)	C21—C20A—C24A—C1	76.1 (3)

C11—C12—C13—C14	−176.1 (4)	O20—C20A—C24A—C24	77.0 (3)
C12—C13—C14—C15	2.1 (6)	C21—C20A—C24A—C24	−42.3 (3)
C13—C14—C15—O29	−17.4 (6)	O20—C20A—C24A—C17A	−43.6 (3)
C13—C14—C15—O16	161.1 (4)	C21—C20A—C24A—C17A	−162.9 (2)
O29—C15—O16—C17	4.3 (5)	C18—C17A—C24A—C1	169.1 (2)
C14—C15—O16—C17	−174.2 (3)	C30—C17A—C24A—C1	−67.3 (3)
C15—O16—C17—C1'	−151.5 (3)	C17—C17A—C24A—C1	61.9 (3)
C15—O16—C17—C17A	93.6 (3)	C18—C17A—C24A—C24	−65.9 (3)
O16—C17—C17A—C18	91.9 (3)	C30—C17A—C24A—C24	57.7 (3)
C1'—C17—C17A—C18	−24.5 (3)	C17—C17A—C24A—C24	−173.1 (2)
O16—C17—C17A—C30	−27.1 (3)	C18—C17A—C24A—C20A	53.6 (3)
C1'—C17—C17A—C30	−143.6 (3)	C30—C17A—C24A—C20A	177.3 (2)
O16—C17—C17A—C24A	−156.7 (2)	C17—C17A—C24A—C20A	−53.6 (3)
C1'—C17—C17A—C24A	86.9 (3)	O8—C7—O27—C10	−2.0 (4)
C30—C17A—C18—O31	36.7 (4)	C6—C7—O27—C10	119.5 (4)
C17—C17A—C18—O31	−85.0 (3)	C11—C10—O27—C7	−144.9 (3)
C24A—C17A—C18—O31	163.0 (3)	C9—C10—O27—C7	−20.5 (4)
C30—C17A—C18—C2'	−35.5 (4)	C19—C18—O31—C2'	117.8 (3)
C17—C17A—C18—C2'	−157.2 (3)	C17A—C18—O31—C2'	−119.1 (3)
C24A—C17A—C18—C2'	90.8 (4)	O20—C19—C1'—C17	−86.6 (3)
C30—C17A—C18—C19	165.4 (2)	C18—C19—C1'—C17	29.5 (3)
C17—C17A—C18—C19	43.8 (3)	O16—C17—C1'—C19	−120.6 (3)
C24A—C17A—C18—C19	−68.2 (3)	C17A—C17—C1'—C19	−2.5 (3)
O31—C18—C19—O20	−155.1 (3)	C19—C18—C2'—O31	−101.1 (3)
C2'—C18—C19—O20	−85.3 (4)	C17A—C18—C2'—O31	104.2 (3)
C17A—C18—C19—O20	74.3 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C30—H30B···O2	0.96	2.36	2.864 (4)	112
C30—H30B···O29	0.96	2.64	3.322 (5)	129
C12—H12···O29	0.93	2.33	2.940 (4)	123
C26—H26C···O25	0.96	2.24	2.989 (5)	134
C1—H1B···O20^{i}	0.97	2.52	3.430 (4)	157
C2'—H2'A···O29^{ii}	0.97	2.63	3.252 (5)	122

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1; (ii) *x*, *y*−1, *z*.

Fig. 1

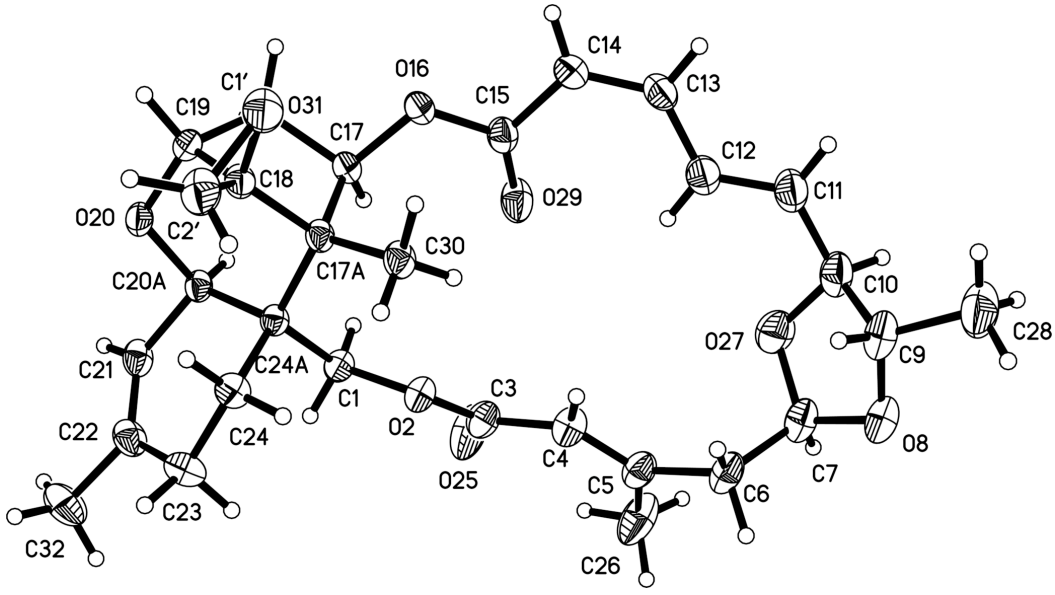
C14
C13
O16
C15
C1′
O31
C19
C17
C12
C18
O29
C11
O20
C2′
C30
C17A
C20A
C10
C28
O27
C9
C21
C24A
C1
C3
C24
O2
C22
C4
O8
O25
C7
C5
C6
C23
C32
C26

Fig. 2