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Crystal structure of a bioactive sesquiterpene isolated from *Artemisia reticulata*

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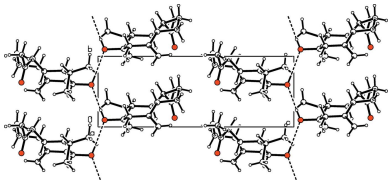
The title compound, $C_{15}H_{24}O_2$ {systematic name: 1-[6-hydroxy-7-(propan-2-yl)-4-methylidene-2,3,3a,4,5,6,7,7a-octahydro-1*H*-inden-1-yl]ethanone} was isolated from *A. reticulata* by column chromatography over silica gel by gradient solvent elution. The molecule comprises a bicyclo[4.3.0]nonane ring bearing acetoxy, hydroxy and isopropyl substituents, and an exocyclic double bond on the cyclohexane ring. In the bicyclic skeleton, the cyclohexane ring adopts a chair conformation ring and the cyclopentane ring is in an envelope conformation. In the crystal, molecules are linked by O—H···O hydrogen bonds, forming chains along [010]. These chains are cross-linked by C—H···O hydrogen bonds.

1. Chemical context

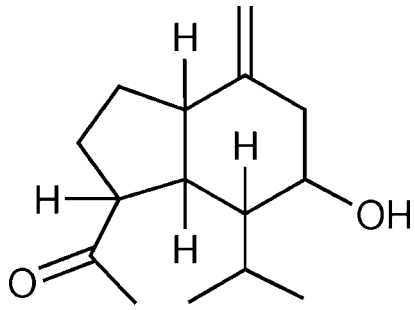
The title compound is a natural product, which has been isolated from the Indian herb *A. reticulata* by column chromatography over silica gel. *A. reticulata* (family: *Asteraceae*) is a traditional herb which has many applications in folklore medicine for conventional therapy against several diseases such as malaria (Klayman *et al.*, 1984; Malagon *et al.*, 1997; Newton & White, 1999), cancer (Efferth *et al.*, 2001; Lai *et al.*, 1995), cardiovascular (Guantai *et al.*, 1999), vasodilatory (Walker, 1996), hepatitis (Aniya *et al.*, 2000) and diabetes (Iriadam *et al.*, 2006). It is found as a constituent in many ayurvedic or herbal drug preparations such as *forkolin* and *Afsanteen* in Indian traditional medicinal systems (Nadkarni, 1954; Satyavati *et al.*, 1987; Subramoniam *et al.*, 1996; Drury, 1978). The *Artemisia* species are a rich source of bioactive sesquiterpenenoids (Klayman *et al.*, 1984) such as artemisinin, artemisin *etc*. Artimisinin and artemisin are secondary metabolites isolated from herbs of the species *A. annua* (Klayman, 1985) belonging to the sesquiterpene class. The title molecule possesses antiplasmodial activity and it is now under clinical trial for the treatment of malaria. Our group are currently searching for artemisin, artemisinin or their analogues from other varieties of *Artemisia* species and as part of these studies, the structure of the title compound is now reported.



2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The compound comprises fused cyclohexane and cyclopentane rings. It has been substantiated by a positive LB test (Liebermann Burchard Test), which indicates that it

belongs to the sesquiterpene class. The compound is soluble in chloroform but has poor solubility in methanol.



The bicyclic skeleton contains one acetyl group at atom C1 of the cyclopentane ring, one isopropyl group and one hydroxyl group located at atoms C6 and C7 in the cyclohexane ring. An exocyclic olefinic double bond is located between atoms C9 and C15 and attached to the cyclohexane ring. The torsion angles C3—C4—C5—C6 and C9—C4—C5—C1 of −169.2 (3) and −170.9 (3)°, respectively, describe the geometry at the junction of the two rings. The C7—C6—C5 and C9—C4—C5 angles are 107.3 (2) and 109.2 (3)°, respectively.

3. Supramolecular features

In the crystal, molecules are linked by O—H···O hydrogen bonds, forming chains along [010] (Table 1 and Fig. 2). These chains are cross-linked by weak C—H···O hydrogen bonds.

4. Database survey

A search of Cambridge Structural Database (CSD, Version 5.36, last update May 2015; Groom & Allen, 2015) found only one molecule, Pulioplopane A (15-hydroxy-10 (14)-oplopen-4-one; Triana *et al.*, 2005) that has a similar structural skeleton to the title sesquitertene although it is is unrelated in a biochemical sense.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···O1^{i}	0.82	2.11	2.927 (4)	175
C11—H11C···O2^{ii}	0.96	2.53	3.430 (6)	157

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

5. Synthesis and crystallization

The title sesquiterpene was isolated as colourless solid from the methanol extract of *A. reticulata* by chromatography over silica gel with a mixture of ethyl acetate and hexane with a gradient elution followed by preparative thin layer chromatography. Crystals were obtained after recrystallization three times from ethyl acetate:hexane (1:4) at room temperature by the slow evaporation method. Bioassay of this molecule has been conducted against human ovarian cancer cell line A 2780 and revealed that it possessed significant antiproliferative activity (unpublished results).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were placed in calculated positions with C—H = 0.93–0.98 Å and O—H = 0.82 Å and refined in a riding-motion approximation with U_{iso}(U) = 1.2U_{eq}(C,O). No Friedel pairs were collected therefore the absolute configuration could not be determined from the X-ray data and the assignment is arbitrary.

Acknowledgements

The authors thank Professor Dr Hartmut, FG Strukturforschung, Material-und Geowissenschaften, Technische Universität Darmstadt, Petersenstress 23, 64287 Darmstadt, and Professor Kingston, Department of Chemistry, M/C 0212, Virginia Polytechnic Institute and State University, Blacks-

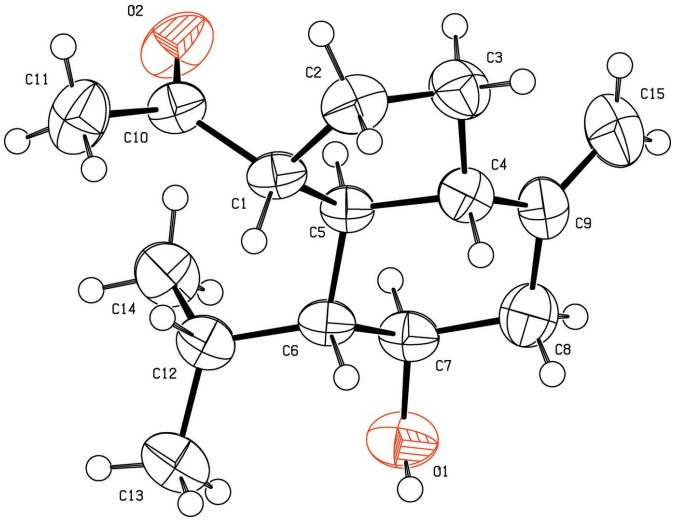


Figure 1
The molecular structure of the title compound, showing 50% probability displacement ellipsoids for non-H atoms.

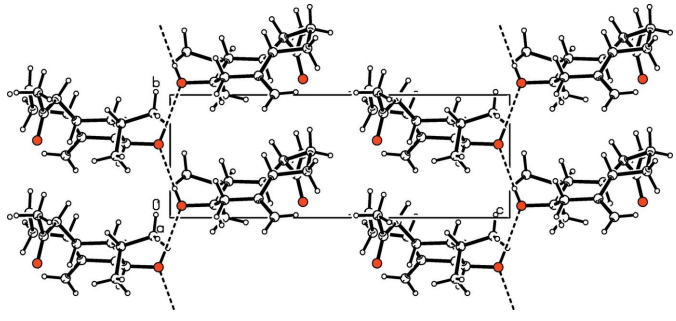


Figure 2
Part of the crystal structure of the title compound, with hydrogen bonds shown as dashed lines.

burg, Virginia 24061, USA, for their kind co-operation to measure diffraction data for the title compound and to carry out an antiproliferative bioassay against cancer cell lines.

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{24}O_2$
M_r	236.34
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	299
a, b, c (Å)	8.849 (4), 5.336 (1), 14.994 (5)
β (°)	99.21 (2)
V (Å^3)	698.9 (4)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.56
Crystal size (mm)	0.50 × 0.18 × 0.15
Data collection	
Diffractometer	Enraf–Nonius CAD-4
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	1916, 1392, 1260
R_{int}	0.052
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.597
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.060, 0.164, 1.10
No. of reflections	1392
No. of parameters	154
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.46, −0.22

Computer programs: *CAD-4-PC* (Enraf–Nonius, 1993), *REDU4* (Stoe & Cie, 1987), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

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Computing details

Data collection: *CAD-4-PC* (Enraf–Nonius, 1993); cell refinement: *CAD-4-PC* (Enraf–Nonius, 1993); data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

1-[6-Hydroxy-7-(propan-2-yl)-4-methylidene-2,3,3a,4,5,6,7,7a-octahydro-1*H*-inden-1-yl]ethanone

Crystal data

$C_{15}H_{24}O_2$
$M_r = 236.34$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 8.849$ (4) Å
$b = 5.336$ (1) Å
$c = 14.994$ (5) Å
$\beta = 99.21$ (2)°
$V = 698.9$ (4) Å^3
$Z = 2$
$F(000) = 260$
$D_x = 1.123$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54180$ Å
Cell parameters from 25 reflections
$\theta = 5.5$–$27.1°$
$\mu = 0.56$ mm^{-1}
$T = 299$ K
Rod, colourless
0.50 × 0.18 × 0.15 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
1916 measured reflections
1392 independent reflections
1260 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 67.0°$, $\theta_{min} = 3.0°$
$h = -10\rightarrow3$
$k = 0\rightarrow6$
$l = -17\rightarrow17$
3 standard reflections every 120 min
intensity decay: 1.0%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.164$
$S = 1.10$
1392 reflections
154 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1147P)^2 + 0.0812P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.46$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 > 2sigma(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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.5467 (3)	0.0974 (5)	0.03391 (14)	0.0580 (7)
H1O	0.5259	0.2380	0.0135	0.070*
O2	0.9664 (3)	0.1293 (5)	0.3910 (2)	0.0680 (8)
C1	0.8020 (3)	0.4666 (6)	0.33401 (19)	0.0401 (7)
H1	0.8184	0.6168	0.2992	0.048*
C2	0.7177 (4)	0.5402 (8)	0.4141 (2)	0.0539 (9)
H2A	0.7821	0.5069	0.4715	0.065*
H2B	0.6912	0.7167	0.4112	0.065*
C3	0.5742 (4)	0.3792 (9)	0.4035 (2)	0.0568 (9)
H3A	0.5943	0.2188	0.4335	0.068*
H3B	0.4923	0.4633	0.4277	0.068*
C4	0.5350 (3)	0.3473 (7)	0.3022 (2)	0.0446 (7)
H4	0.5020	0.5109	0.2765	0.053*
C5	0.6918 (3)	0.2887 (5)	0.27514 (17)	0.0355 (6)
H5	0.7191	0.1174	0.2952	0.043*
C6	0.6880 (3)	0.2967 (5)	0.17229 (17)	0.0370 (7)
H6	0.6501	0.4629	0.1518	0.044*
C7	0.5672 (4)	0.1059 (6)	0.13003 (18)	0.0439 (7)
H7	0.6039	−0.0600	0.1517	0.053*
C8	0.4103 (4)	0.1446 (9)	0.1602 (2)	0.0590 (10)
H8A	0.3654	0.2991	0.1341	0.071*
H8B	0.3429	0.0081	0.1371	0.071*
C9	0.4206 (4)	0.1563 (8)	0.2604 (2)	0.0508 (8)
C10	0.9549 (4)	0.3515 (7)	0.3722 (2)	0.0431 (7)
C11	1.0900 (4)	0.5203 (9)	0.3893 (3)	0.0671 (11)
H11A	1.1664	0.4637	0.3552	0.081*
H11B	1.1313	0.5185	0.4526	0.081*
H11C	1.0594	0.6878	0.3713	0.081*
C12	0.8473 (4)	0.2670 (6)	0.1447 (2)	0.0447 (8)
H12	0.9160	0.3774	0.1847	0.054*
C13	0.8571 (5)	0.3509 (9)	0.0487 (2)	0.0604 (10)
H13A	0.8294	0.5246	0.0418	0.072*
H13B	0.7882	0.2524	0.0067	0.072*
H13C	0.9598	0.3286	0.0371	0.072*

C14	0.9125 (5)	0.0040 (8)	0.1601 (3)	0.0613 (10)
H14A	0.8454	−0.1135	0.1251	0.074*
H14B	0.9217	−0.0377	0.2230	0.074*
H14C	1.0116	−0.0027	0.1419	0.074*
C15	0.3418 (5)	0.0067 (11)	0.3076 (3)	0.0708 (12)
H15A	0.2759	−0.1134	0.2780	0.085*
H15B	0.3528	0.0225	0.3701	0.085*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0792 (15)	0.0505 (15)	0.0419 (11)	−0.0110 (14)	0.0024 (10)	−0.0077 (11)
O2	0.0730 (17)	0.0337 (14)	0.0893 (19)	0.0019 (14)	−0.0110 (13)	0.0124 (14)
C1	0.0543 (16)	0.0251 (14)	0.0392 (13)	−0.0004 (13)	0.0022 (12)	0.0020 (12)
C2	0.067 (2)	0.045 (2)	0.0479 (16)	0.0059 (17)	0.0046 (14)	−0.0101 (16)
C3	0.0614 (19)	0.063 (2)	0.0489 (17)	0.0040 (18)	0.0176 (14)	−0.0047 (18)
C4	0.0501 (16)	0.0376 (17)	0.0472 (16)	0.0042 (15)	0.0112 (12)	−0.0022 (14)
C5	0.0451 (14)	0.0226 (14)	0.0386 (14)	−0.0002 (12)	0.0059 (11)	0.0015 (12)
C6	0.0513 (16)	0.0226 (14)	0.0369 (13)	0.0002 (13)	0.0064 (11)	0.0013 (12)
C7	0.0570 (17)	0.0330 (17)	0.0410 (14)	−0.0066 (15)	0.0052 (13)	−0.0001 (14)
C8	0.0527 (18)	0.062 (3)	0.0603 (19)	−0.010 (2)	0.0022 (14)	−0.004 (2)
C9	0.0423 (15)	0.049 (2)	0.0626 (18)	−0.0012 (16)	0.0135 (13)	−0.0002 (17)
C10	0.0516 (17)	0.0324 (16)	0.0438 (15)	−0.0007 (14)	0.0026 (12)	−0.0008 (14)
C11	0.0541 (19)	0.047 (2)	0.095 (3)	−0.0055 (18)	−0.0023 (18)	−0.002 (2)
C12	0.0551 (17)	0.0307 (16)	0.0492 (17)	−0.0035 (15)	0.0108 (13)	−0.0007 (14)
C13	0.078 (2)	0.052 (2)	0.0559 (19)	−0.004 (2)	0.0248 (17)	−0.0006 (18)
C14	0.070 (2)	0.042 (2)	0.077 (2)	0.0144 (19)	0.0264 (18)	0.0068 (19)
C15	0.060 (2)	0.076 (3)	0.080 (2)	−0.014 (2)	0.0229 (18)	−0.004 (2)

Geometric parameters (Å, º)

O1—C7	1.424 (3)	C7—C8	1.542 (5)
O1—H1O	0.8200	C7—H7	0.9800
O2—C10	1.219 (5)	C8—C9	1.493 (5)
C1—C10	1.513 (4)	C8—H8A	0.9700
C1—C5	1.535 (4)	C8—H8B	0.9700
C1—C2	1.562 (5)	C9—C15	1.335 (6)
C1—H1	0.9800	C10—C11	1.486 (5)
C2—C3	1.521 (6)	C11—H11A	0.9600
C2—H2A	0.9700	C11—H11B	0.9600
C2—H2B	0.9700	C11—H11C	0.9600
C3—C4	1.513 (4)	C12—C14	1.521 (5)
C3—H3A	0.9700	C12—C13	1.523 (5)
C3—H3B	0.9700	C12—H12	0.9800
C4—C9	1.501 (5)	C13—H13A	0.9600
C4—C5	1.539 (4)	C13—H13B	0.9600
C4—H4	0.9800	C13—H13C	0.9600
C5—C6	1.538 (3)	C14—H14A	0.9600

C5—H5	0.9800	C14—H14B	0.9600
C6—C7	1.537 (4)	C14—H14C	0.9600
C6—C12	1.540 (4)	C15—H15A	0.9300
C6—H6	0.9800	C15—H15B	0.9300

C7—O1—H1O	109.5	C6—C7—H7	106.8
C10—C1—C5	114.5 (3)	C8—C7—H7	106.8
C10—C1—C2	108.6 (2)	C9—C8—C7	112.9 (3)
C5—C1—C2	105.1 (2)	C9—C8—H8A	109.0
C10—C1—H1	109.5	C7—C8—H8A	109.0
C5—C1—H1	109.5	C9—C8—H8B	109.0
C2—C1—H1	109.5	C7—C8—H8B	109.0
C3—C2—C1	105.8 (3)	H8A—C8—H8B	107.8
C3—C2—H2A	110.6	C15—C9—C8	123.8 (4)
C1—C2—H2A	110.6	C15—C9—C4	124.0 (4)
C3—C2—H2B	110.6	C8—C9—C4	112.2 (3)
C1—C2—H2B	110.6	O2—C10—C11	121.0 (3)
H2A—C2—H2B	108.7	O2—C10—C1	121.3 (3)
C4—C3—C2	102.8 (3)	C11—C10—C1	117.7 (3)
C4—C3—H3A	111.2	C10—C11—H11A	109.5
C2—C3—H3A	111.2	C10—C11—H11B	109.5
C4—C3—H3B	111.2	H11A—C11—H11B	109.5
C2—C3—H3B	111.2	C10—C11—H11C	109.5
H3A—C3—H3B	109.1	H11A—C11—H11C	109.5
C9—C4—C3	121.8 (3)	H11B—C11—H11C	109.5
C9—C4—C5	109.2 (3)	C14—C12—C13	109.7 (3)
C3—C4—C5	102.5 (2)	C14—C12—C6	113.3 (3)
C9—C4—H4	107.5	C13—C12—C6	114.6 (3)
C3—C4—H4	107.5	C14—C12—H12	106.2
C5—C4—H4	107.5	C13—C12—H12	106.2
C1—C5—C6	118.0 (2)	C6—C12—H12	106.2
C1—C5—C4	103.8 (2)	C12—C13—H13A	109.5
C6—C5—C4	112.5 (2)	C12—C13—H13B	109.5
C1—C5—H5	107.3	H13A—C13—H13B	109.5
C6—C5—H5	107.3	C12—C13—H13C	109.5
C4—C5—H5	107.3	H13A—C13—H13C	109.5
C7—C6—C5	107.3 (2)	H13B—C13—H13C	109.5
C7—C6—C12	115.3 (3)	C12—C14—H14A	109.5
C5—C6—C12	113.1 (2)	C12—C14—H14B	109.5
C7—C6—H6	106.9	H14A—C14—H14B	109.5
C5—C6—H6	106.9	C12—C14—H14C	109.5
C12—C6—H6	106.9	H14A—C14—H14C	109.5
O1—C7—C6	113.9 (2)	H14B—C14—H14C	109.5
O1—C7—C8	109.0 (2)	C9—C15—H15A	120.0
C6—C7—C8	112.9 (3)	C9—C15—H15B	120.0
O1—C7—H7	106.8	H15A—C15—H15B	120.0

C10—C1—C2—C3	−116.4 (3)	C5—C6—C7—C8	52.9 (3)

C5—C1—C2—C3	6.5 (4)	C12—C6—C7—C8	179.9 (3)
C1—C2—C3—C4	−31.5 (4)	O1—C7—C8—C9	−179.9 (3)
C2—C3—C4—C9	166.7 (3)	C6—C7—C8—C9	−52.2 (4)
C2—C3—C4—C5	44.5 (4)	C7—C8—C9—C15	−124.2 (4)
C10—C1—C5—C6	−95.1 (3)	C7—C8—C9—C4	53.1 (4)
C2—C1—C5—C6	145.9 (3)	C3—C4—C9—C15	2.1 (6)
C10—C1—C5—C4	139.6 (3)	C5—C4—C9—C15	121.1 (4)
C2—C1—C5—C4	20.5 (3)	C3—C4—C9—C8	−175.3 (3)
C9—C4—C5—C1	−170.9 (3)	C5—C4—C9—C8	−56.3 (4)
C3—C4—C5—C1	−40.5 (3)	C5—C1—C10—O2	−31.7 (5)
C9—C4—C5—C6	60.4 (3)	C2—C1—C10—O2	85.3 (4)
C3—C4—C5—C6	−169.2 (3)	C5—C1—C10—C11	150.5 (3)
C1—C5—C6—C7	−179.0 (3)	C2—C1—C10—C11	−92.5 (4)
C4—C5—C6—C7	−58.0 (3)	C7—C6—C12—C14	−53.3 (4)
C1—C5—C6—C12	52.8 (3)	C5—C6—C12—C14	70.7 (4)
C4—C5—C6—C12	173.7 (3)	C7—C6—C12—C13	73.6 (4)
C5—C6—C7—O1	178.0 (2)	C5—C6—C12—C13	−162.4 (3)
C12—C6—C7—O1	−55.0 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O1^{i}	0.82	2.11	2.927 (4)	175
C11—H11*C*···O2^{ii}	0.96	2.53	3.430 (6)	157

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