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(1*R*,4*S*,8*R*,12*S*,13*S*,14*R*,16*S*,19*R*)-14-Hydroxy-7,7-dimethyl-17-methylene-2,9,18-trioxo-3,10-dioxapentacyclo-[14.2.1.0^{1,13}.0^{4,12}.0^{8,12}]nonadec-19-yl acetate

Hao Shi

College of Pharmaceutical Science, Zhejiang University of Technology, Hangzhou 310014, People's Republic of China
Correspondence e-mail: shihao@zjut.edu.cn

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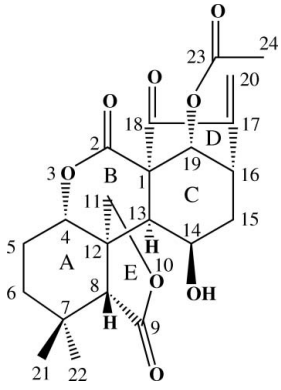
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.051; wR factor = 0.115; data-to-parameter ratio = 8.5.

The title compound, $C_{22}H_{26}O_8$, prepared from the natural diterpenoid Macrocalyxin J, is built up from five fused rings. Cyclohenane ring *A* adopts a chair conformation, ring *B* exists in a screw-boat conformation and ring *C* adopts a boat conformation; the two five membered rings adopt envelope conformations. Two unique molecules are present in the asymmetric unit; both independent molecules have the same absolute configuration, the absolute configuration being deduced from the chirality of Macrocalyxin A, which was isolated from the same plant (*i.e. Rabdosia macrocalyx*) as Macrocalyxin J. The crystal structure displays intermolecular O—H···O hydrogen bonds.

Related literature

For related literature, see: Cremer & Pople (1975); Shi *et al.* (2003, 2007); Wang *et al.* (1984).



Experimental

Crystal data

$C_{22}H_{26}O_8$
M_r = 418.43
Orthorhombic, $P2_12_12_1$
a = 12.0055 (11) Å
b = 13.5835 (13) Å
c = 25.027 (2) Å
V = 4081.3 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.49 × 0.43 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.744, T_{max} = 1.000
(expected range = 0.720–0.968)
24111 measured reflections
4945 independent reflections
3810 reflections with $I > 2\sigma(I)$
R_{int} = 0.130

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.115
S = 1.00
4945 reflections
583 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 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
O28—H28*A*···O1^{i}	0.81 (2)	1.93 (2)	2.711 (3)	161 (4)
O4—H4*A*···O26	0.84 (2)	2.20 (3)	2.957 (4)	150 (4)

Symmetry code: (i) $x+1, y, z$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2053).

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supplementary materials

Acta Cryst. (2007). E**63**, o4439 [**doi:10.1107/S1600536807052099**]

(1*R*,4*S*,8*R*,12*S*,13*S*,14*R*,16*S*,19*R*)-14-Hydroxy-7,7-dimethyl-17-methylene-2,9,18-trioxo-3,10-dioxapentacyclo[14.2.1.$0^{1,13}$.$0^{4,12}$.$0^{8,12}$]nonadec-19-yl acetate

H. Shi

Comment

Since the natural diterpenoid Macrocalyxin J exhibits cytotoxicity *in vitro* against cultures of Hela cells and the IC_{50} =31.597μg/ml (Shi *et al.*, 2007), we have derived the title compound from it.

The crystal packing is shown in Fig. 3. Two unique molecules are present in the asymmetric unit, both molecule 1 (Fig.1) and molecule 2 (Fig.2) are built up from five fused rings, three six membered and two five membered rings. Some geometrical features of these rings were investigated using *PLATON* (Spek, 2003).

For the molecule 1, cyclohexane ring A (C4—C8/C12) adopts a chair conformation with puckering parameters (Cremer & Pople, 1975) Q = 0.5295 (42) Å, and θ= 157.69 (43) and φ = 271.5 (11) °, ring B (O3/C2/C1/C13/C12/C4) exists in a screw-boat conformation (Q = 0.6672 (33) Å, θ = 108.66 (28) and φ = 92.0 (3) °), ring C (C1/C13—C16/C19) adopt the boat conformation (Q = 0.8109 (35) Å, θ = 79.21 (24) and φ = 294.2 (2) °). The two five-membered rings, ring D (C1/C18/C17/C16/C19) adopts an envelope conformation with puckering parameters Q2 = 0.4565 (34) Å, and φ2 = 143.6 (4)° (envelope on C19), the ring E (O10/C9/C8/C12/C11) adopts an envelope conformation with puckering parameters Q2 = 0.3341 (36) Å, and φ2 = 284.7 (6)° (envelope on C12).

For the molecule 2, cyclohexane ring A' (C28—C32/C36) adopts a chair conformation with puckering parameters Q = 0.5312 (40) Å, and θ= 156.14 (41) and φ =274.4 (10) °, ring B' (O27/C26/C25/C37/C36/C28) exists in a screw-boat conformation (Q = 0.6421 (36) Å, and θ= 110.70 (31) and φ =94.7 (3) °), ring C' (C25/C37—C40/C43) adopt the boat conformation (Q = 0.8400 (37) Å, θ = 80.52 (25) and φ = 293.6 (3)°). The two five-membered rings, ring D' (C25/C42/C41/C40/C43) adopts an envelope conformation with puckering parameters Q2 = 0.4526 (38) Å, and φ2 = 146.0 (5)° (envelope on C43), the ring E' (O34/C33/C32/C36/C35) adopts an envelope conformation with puckering parameters Q2 = 0.3156 (35) Å, and φ2 = 284.8 (6) ° (envelope on C36).

Since the title compound was prepared from Macrocalyxin J, which was isolated from the same plant (*i.e. Rabdosia macrocalyx*) as Macrocalyxin A, the configuration can be deduced from the known chirality of the Macrocalyxin A (Shi *et al.*, 2003),and thus Fig. 1 and Fig. 2 represents the correct absolute configuration.

Experimental

Cooling in ice-water bath, 0.2 ml Jones reagent was added to a solution of Macrocalyxin J (200 mg; isolated from *Rabdosia macrocalyx*) in acetone (8 ml), after stirring for 20 minutes, filtrated and the solution was added 120 ml 15% $NaHCO_3$ in water, the mixture extracted 3 times with 90 ml diethyl ether, after evaporation of the solvent, a white residue was gained. Recrystallization with methanol gave the title compound as colorless crystals.

Crystals suitable for X-ray structure analysis were obtained by slow evaporation from a solution of methanol at room temperature.

Refinement

H atoms bonded to O atoms and some H atoms bonded to CH were located in a difference map, and with *U*iso~(H) = 1.2*U*~eq~(O, C). Other H atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.96 Å (CH_3), 0.97 Å (CH_2) and 0.98(CH) and with the temperature factors U_{iso}= 1.5 U_{eq}(CH_3) and 1.2 U_{eq}(CH_2, CH). Both independent molecules have the same absolute configuration, although this could not be determined reliably from the X-ray data and Friedel reflections were merged.

Figures

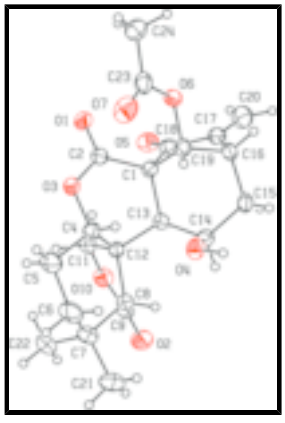

Fig. 1. Perspective view of molecule 1 of the title compound, shown with 30% probability displacement ellipsoids.

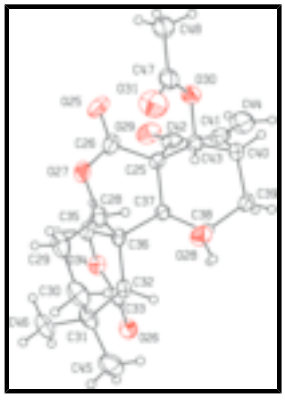

Fig. 2. Perspective view of molecule 2 of the title compound, shown with 30% probability displacement ellipsoids.

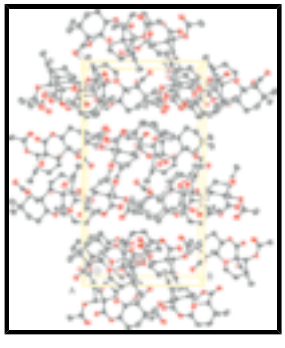

Fig. 3. The crystal packing diagram for the title compound viewed normal to the (100) plane. H atoms have been omitted for clarity.

(1*R*,4*S*,8*R*,12*S*,13*S*,14*R*,16*S*, 19*R*)-14-Hydroxy-7,7-dimethyl-17-methylene-2,9,18-trioxo-3,10-dioxapentacyclo[14.2.1.0^{1,13}.0^{4,12}.0^{8,12}]nonadec-19-yl acetate

Crystal data

$C_{22}H_{26}O_8$	F_{000} = 1776
M_r = 418.43	D_x = 1.362 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 5228 reflections
a = 12.0055 (11) Å	θ = 4.7–43.5º
b = 13.5835 (13) Å	μ = 0.10 mm^{-1}
c = 25.027 (2) Å	T = 293 (2) K
V = 4081.3 (6) Å^3	Prismatic, colorless
Z = 8	0.49 × 0.43 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer	4945 independent reflections
Radiation source: fine-focus sealed tube	3810 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.130
T = 293(2) K	θ_{max} = 27.0º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Bruker, 1999)	h = −13→15
T_{min} = 0.744, T_{max} = 1.000	k = −16→17
24111 measured reflections	l = −31→30

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.051	$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.115	$(\Delta/\sigma)_{max} < 0.001$
S = 1.00	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
4945 reflections	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
583 parameters	Extinction correction: none
5 restraints	
Primary atom site location: structure-invariant direct methods	
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}
O1	−0.0773 (2)	0.39858 (19)	0.15867 (9)	0.0571 (7)
O2	0.0191 (3)	−0.0582 (2)	0.03545 (10)	0.0745 (9)
O3	0.0225 (2)	0.27304 (16)	0.18225 (8)	0.0443 (5)
O4	0.2759 (2)	0.22386 (19)	0.08037 (10)	0.0505 (6)
O5	−0.1365 (2)	0.36138 (18)	0.04604 (10)	0.0557 (6)
O6	0.1069 (2)	0.50275 (16)	0.10433 (8)	0.0479 (6)
O7	0.1822 (3)	0.4751 (2)	0.18441 (10)	0.0726 (8)
O10	−0.0833 (2)	0.05219 (18)	0.07849 (10)	0.0533 (6)
O25	0.4868 (2)	0.8092 (2)	0.15326 (11)	0.0702 (8)
O26	0.4933 (2)	0.31505 (19)	0.05534 (9)	0.0564 (7)
O27	0.5162 (2)	0.66457 (19)	0.18918 (9)	0.0559 (7)
O28	0.7958 (2)	0.5540 (2)	0.12833 (11)	0.0574 (7)
O29	0.4717 (2)	0.7662 (2)	0.03890 (11)	0.0700 (8)
O30	0.7150 (2)	0.85219 (17)	0.12142 (9)	0.0535 (6)
O31	0.7390 (3)	0.8188 (3)	0.20754 (12)	0.0931 (11)
O34	0.41033 (18)	0.45354 (18)	0.07968 (8)	0.0470 (6)
C1	0.0423 (3)	0.3345 (2)	0.09064 (11)	0.0359 (7)
C2	−0.0100 (3)	0.3384 (2)	0.14598 (12)	0.0395 (7)
C4	0.1025 (3)	0.1989 (2)	0.16628 (12)	0.0412 (8)
H4	0.1748	0.2301	0.1596	0.049*
C5	0.1133 (4)	0.1263 (3)	0.21173 (13)	0.0585 (10)
H5A	0.0404	0.1013	0.2216	0.070*
H5B	0.1458	0.1583	0.2427	0.070*
C6	0.1873 (4)	0.0425 (3)	0.19322 (16)	0.0671 (11)
H6A	0.2034	0.0002	0.2235	0.081*
H6B	0.2573	0.0695	0.1806	0.081*
C7	0.1356 (3)	−0.0193 (3)	0.14880 (15)	0.0572 (10)
C8	0.1063 (3)	0.0509 (2)	0.10027 (13)	0.0432 (8)
C9	0.0142 (3)	0.0071 (3)	0.06754 (13)	0.0507 (9)
C11	−0.0653 (3)	0.1293 (2)	0.11657 (12)	0.0428 (8)
H11A	−0.0862	0.1076	0.1521	0.051*
H11B	−0.1092	0.1868	0.1074	0.051*
C12	0.0589 (2)	0.1534 (2)	0.11442 (11)	0.0345 (7)

C13	0.0763 (3)	0.2297 (2)	0.06897 (11)	0.0336 (6)
H13	0.0215	0.2132	0.0414	0.040*
C14	0.1898 (3)	0.2287 (2)	0.04108 (12)	0.0413 (7)
H14	0.1941	0.1690	0.0192	0.050*
C15	0.2046 (3)	0.3179 (2)	0.00380 (12)	0.0448 (8)
H15A	0.1711	0.3027	−0.0305	0.054*
H15B	0.2836	0.3285	−0.0020	0.054*
C16	0.1526 (3)	0.4140 (2)	0.02532 (12)	0.0426 (8)
H16	0.1971	0.4716	0.0152	0.051*
C17	0.0344 (3)	0.4247 (2)	0.00754 (12)	0.0481 (9)
C18	−0.0376 (3)	0.3743 (2)	0.04759 (12)	0.0415 (8)
C19	0.1400 (3)	0.4067 (2)	0.08557 (12)	0.0411 (8)
C20	−0.0059 (4)	0.4687 (3)	−0.03553 (14)	0.0744 (13)
H20A	−0.0823	0.4690	−0.0418	0.089*
H20B	0.0421	0.4992	−0.0595	0.089*
C21	0.2210 (4)	−0.0943 (3)	0.12855 (19)	0.0821 (14)
H21A	0.2889	−0.0610	0.1195	0.123*
H21B	0.1921	−0.1270	0.0975	0.123*
H21C	0.2355	−0.1420	0.1560	0.123*
C22	0.0342 (4)	−0.0769 (3)	0.16967 (17)	0.0720 (12)
H22A	0.0558	−0.1156	0.2000	0.108*
H22B	0.0067	−0.1195	0.1420	0.108*
H22C	−0.0232	−0.0315	0.1800	0.108*
C23	0.1326 (3)	0.5276 (3)	0.15509 (14)	0.0525 (9)
C24	0.0901 (5)	0.6276 (3)	0.16802 (16)	0.0821 (15)
H24A	0.1184	0.6478	0.2022	0.123*
H24B	0.0102	0.6264	0.1691	0.123*
H24C	0.1143	0.6732	0.1411	0.123*
C25	0.6069 (3)	0.7044 (2)	0.10372 (12)	0.0377 (7)
C26	0.5321 (3)	0.7303 (3)	0.14997 (14)	0.0497 (9)
C28	0.5763 (3)	0.5727 (3)	0.18558 (12)	0.0458 (8)
C29	0.5426 (3)	0.5069 (3)	0.23096 (12)	0.0622 (11)
H29A	0.4624	0.4978	0.2309	0.075*
H29B	0.5637	0.5365	0.2647	0.075*
C30	0.6000 (4)	0.4088 (3)	0.22445 (13)	0.0653 (11)
H30A	0.5882	0.3698	0.2564	0.078*
H30B	0.6795	0.4196	0.2207	0.078*
C31	0.5579 (3)	0.3511 (3)	0.17602 (13)	0.0532 (9)
C32	0.5758 (3)	0.4175 (2)	0.12488 (12)	0.0396 (7)
C33	0.4935 (3)	0.3876 (2)	0.08301 (12)	0.0420 (8)
C35	0.4291 (3)	0.5328 (3)	0.11635 (12)	0.0438 (8)
H35A	0.3837	0.5247	0.1481	0.053*
H35B	0.4109	0.5954	0.0999	0.053*
C36	0.5532 (2)	0.5285 (2)	0.13060 (11)	0.0361 (7)
C37	0.6168 (3)	0.5915 (2)	0.08923 (11)	0.0345 (7)
H37	0.5773	0.5829	0.0553	0.041*
C38	0.7378 (3)	0.5607 (3)	0.07876 (13)	0.0439 (8)
C39	0.7965 (3)	0.6321 (2)	0.04099 (14)	0.0517 (9)
H39A	0.7759	0.6163	0.0045	0.062*

H39B	0.8763	0.6232	0.0443	0.062*
C40	0.7676 (3)	0.7411 (3)	0.05215 (14)	0.0485 (9)
C41	0.6689 (3)	0.7737 (3)	0.02033 (13)	0.0539 (9)
C42	0.5664 (3)	0.7532 (3)	0.05151 (13)	0.0488 (9)
C43	0.7246 (3)	0.7493 (2)	0.10914 (13)	0.0413 (8)
C44	0.6660 (5)	0.8120 (3)	−0.02801 (16)	0.0833 (15)
H44A	0.5980	0.8272	−0.0438	0.100*
H44B	0.7320	0.8239	−0.0464	0.100*
C45	0.6298 (4)	0.2586 (3)	0.16936 (19)	0.0791 (13)
H45A	0.7057	0.2775	0.1630	0.119*
H45B	0.6030	0.2209	0.1396	0.119*
H45C	0.6258	0.2196	0.2013	0.119*
C46	0.4377 (4)	0.3195 (3)	0.18463 (14)	0.0650 (12)
H46A	0.4316	0.2851	0.2180	0.097*
H46B	0.4151	0.2769	0.1560	0.097*
H46C	0.3906	0.3766	0.1853	0.097*
C47	0.7231 (4)	0.8770 (3)	0.17307 (16)	0.0588 (10)
C48	0.7040 (4)	0.9838 (3)	0.18026 (18)	0.0796 (13)
H48A	0.6256	0.9972	0.1787	0.119*
H48B	0.7413	1.0194	0.1524	0.119*
H48C	0.7328	1.0040	0.2143	0.119*
H8	0.171 (3)	0.063 (2)	0.0796 (13)	0.049 (10)*
H19	0.2078 (18)	0.385 (2)	0.1015 (10)	0.031 (8)*
H28	0.6554 (17)	0.589 (2)	0.1872 (12)	0.045 (9)*
H32	0.653 (3)	0.402 (2)	0.1139 (13)	0.048 (9)*
H38	0.740 (3)	0.495 (3)	0.0650 (11)	0.037 (8)*
H40	0.830 (3)	0.783 (3)	0.0480 (13)	0.048 (10)*
H43	0.768 (3)	0.714 (3)	0.1363 (14)	0.055 (10)*
H4A	0.336 (3)	0.234 (4)	0.0637 (16)	0.096 (18)*
H28A	0.840 (3)	0.509 (3)	0.1307 (17)	0.084 (16)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0640 (16)	0.0566 (15)	0.0508 (13)	0.0240 (14)	0.0136 (13)	0.0077 (12)
O2	0.110 (2)	0.0536 (16)	0.0604 (16)	0.0009 (16)	0.0056 (17)	−0.0162 (14)
O3	0.0565 (14)	0.0448 (13)	0.0315 (11)	0.0066 (11)	0.0022 (10)	0.0021 (10)
O4	0.0360 (13)	0.0637 (15)	0.0517 (13)	0.0011 (12)	0.0020 (12)	0.0048 (13)
O5	0.0457 (15)	0.0590 (16)	0.0624 (15)	0.0119 (12)	−0.0150 (13)	−0.0013 (12)
O6	0.0733 (17)	0.0365 (12)	0.0339 (11)	0.0004 (11)	−0.0012 (11)	−0.0007 (10)
O7	0.083 (2)	0.093 (2)	0.0417 (14)	0.0110 (18)	−0.0144 (14)	−0.0084 (15)
O10	0.0526 (15)	0.0511 (14)	0.0562 (14)	−0.0107 (12)	−0.0047 (12)	−0.0043 (12)
O25	0.0668 (18)	0.0666 (18)	0.0772 (18)	0.0206 (15)	0.0115 (15)	−0.0222 (15)
O26	0.0671 (17)	0.0567 (15)	0.0454 (13)	−0.0126 (13)	0.0045 (12)	−0.0114 (12)
O27	0.0620 (16)	0.0645 (16)	0.0412 (13)	−0.0083 (14)	0.0183 (12)	−0.0139 (12)
O28	0.0497 (15)	0.0595 (17)	0.0629 (15)	0.0171 (13)	−0.0058 (13)	0.0107 (13)
O29	0.0652 (18)	0.0711 (18)	0.0738 (18)	0.0248 (15)	−0.0267 (15)	0.0011 (15)
O30	0.0673 (17)	0.0458 (14)	0.0473 (14)	−0.0076 (12)	0.0056 (13)	−0.0067 (11)

O31	0.135 (3)	0.092 (2)	0.0515 (16)	−0.015 (2)	−0.0051 (19)	−0.0069 (17)
O34	0.0410 (13)	0.0589 (14)	0.0412 (12)	−0.0056 (12)	−0.0066 (11)	−0.0046 (11)
C1	0.0360 (17)	0.0395 (17)	0.0321 (15)	0.0055 (13)	−0.0008 (13)	0.0000 (13)
C2	0.0398 (18)	0.0377 (17)	0.0409 (17)	0.0007 (15)	0.0008 (15)	0.0005 (14)
C4	0.0382 (18)	0.0461 (19)	0.0392 (16)	0.0067 (14)	−0.0008 (14)	0.0015 (14)
C5	0.077 (3)	0.057 (2)	0.0414 (18)	0.008 (2)	−0.0172 (19)	0.0046 (17)
C6	0.070 (3)	0.063 (3)	0.067 (2)	0.018 (2)	−0.018 (2)	0.018 (2)
C7	0.067 (2)	0.047 (2)	0.058 (2)	0.0143 (18)	−0.0004 (19)	0.0117 (18)
C8	0.047 (2)	0.0361 (17)	0.0466 (18)	0.0042 (15)	0.0088 (16)	0.0007 (15)
C9	0.070 (3)	0.0391 (18)	0.0431 (18)	0.0007 (18)	0.0051 (18)	0.0033 (16)
C11	0.0416 (19)	0.0459 (18)	0.0411 (17)	−0.0027 (15)	0.0021 (15)	0.0022 (15)
C12	0.0320 (16)	0.0368 (16)	0.0348 (15)	0.0039 (13)	0.0011 (13)	0.0035 (13)
C13	0.0340 (16)	0.0345 (15)	0.0324 (15)	−0.0001 (13)	−0.0031 (13)	0.0000 (13)
C14	0.0416 (18)	0.0423 (18)	0.0401 (17)	−0.0008 (15)	0.0018 (14)	−0.0026 (14)
C15	0.048 (2)	0.0512 (19)	0.0353 (16)	−0.0026 (16)	0.0084 (15)	0.0010 (15)
C16	0.056 (2)	0.0376 (18)	0.0343 (16)	−0.0083 (16)	0.0053 (15)	0.0036 (14)
C17	0.068 (2)	0.0427 (19)	0.0341 (16)	0.0077 (17)	−0.0025 (16)	0.0008 (15)
C18	0.048 (2)	0.0390 (18)	0.0374 (17)	0.0097 (15)	−0.0080 (16)	−0.0044 (14)
C19	0.046 (2)	0.0443 (19)	0.0328 (16)	−0.0012 (16)	−0.0011 (15)	−0.0008 (15)
C20	0.100 (4)	0.081 (3)	0.042 (2)	0.018 (3)	−0.005 (2)	0.012 (2)
C21	0.091 (3)	0.062 (3)	0.093 (3)	0.035 (3)	0.001 (3)	0.015 (2)
C22	0.095 (3)	0.052 (2)	0.069 (2)	0.006 (2)	0.011 (2)	0.021 (2)
C23	0.061 (2)	0.058 (2)	0.0383 (18)	−0.0153 (19)	0.0054 (18)	−0.0045 (18)
C24	0.136 (5)	0.057 (3)	0.053 (2)	−0.005 (3)	0.021 (3)	−0.015 (2)
C25	0.0400 (18)	0.0402 (17)	0.0328 (15)	0.0067 (14)	0.0001 (13)	−0.0017 (13)
C26	0.0374 (18)	0.062 (2)	0.050 (2)	−0.0009 (17)	0.0043 (16)	−0.0174 (19)
C28	0.042 (2)	0.059 (2)	0.0361 (17)	−0.0106 (17)	0.0028 (15)	−0.0047 (15)
C29	0.070 (3)	0.089 (3)	0.0279 (16)	−0.030 (2)	0.0043 (16)	−0.0071 (18)
C30	0.077 (3)	0.082 (3)	0.0372 (19)	−0.020 (2)	−0.0132 (19)	0.0215 (19)
C31	0.057 (2)	0.061 (2)	0.0416 (18)	−0.0136 (18)	−0.0032 (17)	0.0192 (17)
C32	0.0357 (18)	0.0476 (19)	0.0355 (16)	−0.0014 (15)	0.0037 (14)	0.0045 (14)
C33	0.047 (2)	0.0493 (19)	0.0299 (15)	−0.0111 (17)	0.0080 (15)	0.0020 (15)
C35	0.0357 (17)	0.056 (2)	0.0396 (16)	−0.0025 (16)	0.0030 (14)	−0.0084 (15)
C36	0.0341 (17)	0.0466 (19)	0.0275 (14)	−0.0026 (14)	0.0019 (13)	−0.0008 (13)
C37	0.0396 (17)	0.0356 (16)	0.0283 (14)	0.0022 (13)	0.0016 (13)	0.0023 (13)
C38	0.0423 (19)	0.0420 (19)	0.0475 (19)	0.0059 (15)	0.0089 (16)	0.0034 (16)
C39	0.050 (2)	0.047 (2)	0.058 (2)	0.0120 (17)	0.0213 (18)	0.0034 (17)
C40	0.050 (2)	0.045 (2)	0.051 (2)	−0.0025 (17)	0.0159 (17)	0.0020 (16)
C41	0.080 (3)	0.0402 (19)	0.0413 (19)	0.0109 (19)	0.0048 (18)	0.0008 (15)
C42	0.061 (2)	0.0403 (19)	0.0456 (18)	0.0118 (17)	−0.0118 (18)	0.0004 (15)
C43	0.0422 (19)	0.0413 (19)	0.0403 (17)	0.0033 (15)	0.0008 (15)	0.0009 (15)
C44	0.121 (4)	0.073 (3)	0.056 (2)	0.013 (3)	0.010 (3)	0.021 (2)
C45	0.086 (3)	0.068 (3)	0.083 (3)	0.002 (2)	−0.011 (3)	0.030 (2)
C46	0.070 (3)	0.079 (3)	0.045 (2)	−0.027 (2)	0.0018 (19)	0.0154 (19)
C47	0.061 (2)	0.059 (2)	0.056 (2)	−0.019 (2)	0.008 (2)	−0.014 (2)
C48	0.086 (3)	0.070 (3)	0.082 (3)	−0.023 (2)	0.024 (3)	−0.026 (2)

Geometric parameters (Å, °)

O1—C2	1.193 (4)	C20—H20A	0.9300
O2—C9	1.199 (4)	C20—H20B	0.9300
O3—C2	1.328 (4)	C21—H21A	0.9600
O3—C4	1.447 (4)	C21—H21B	0.9600
O4—C14	1.428 (4)	C21—H21C	0.9600
O4—H4A	0.84 (2)	C22—H22A	0.9600
O5—C18	1.201 (4)	C22—H22B	0.9600
O6—C23	1.350 (4)	C22—H22C	0.9600
O6—C19	1.442 (4)	C23—C24	1.487 (6)
O7—C23	1.184 (4)	C24—H24A	0.9600
O10—C9	1.348 (5)	C24—H24B	0.9600
O10—C11	1.432 (4)	C24—H24C	0.9600
O25—C26	1.204 (4)	C25—C26	1.507 (5)
O26—C33	1.205 (4)	C25—C42	1.544 (4)
O27—C26	1.340 (4)	C25—C43	1.544 (5)
O27—C28	1.444 (5)	C25—C37	1.581 (4)
O28—C38	1.426 (4)	C28—C29	1.501 (5)
O28—H28A	0.81 (2)	C28—C36	1.526 (4)
O29—C42	1.193 (4)	C28—H28	0.976 (18)
O30—C47	1.339 (4)	C29—C30	1.509 (6)
O30—C43	1.436 (4)	C29—H29A	0.9700
O31—C47	1.185 (5)	C29—H29B	0.9700
O34—C33	1.344 (4)	C30—C31	1.529 (5)
O34—C35	1.433 (4)	C30—H30A	0.9700
C1—C2	1.521 (4)	C30—H30B	0.9700
C1—C19	1.534 (5)	C31—C46	1.521 (6)
C1—C18	1.540 (4)	C31—C45	1.534 (6)
C1—C13	1.578 (4)	C31—C32	1.580 (4)
C4—C5	1.511 (5)	C32—C33	1.495 (5)
C4—C12	1.530 (4)	C32—C36	1.540 (5)
C4—H4	0.9800	C32—H32	0.99 (4)
C5—C6	1.517 (6)	C35—C36	1.533 (4)
C5—H5A	0.9700	C35—H35A	0.9700
C5—H5B	0.9700	C35—H35B	0.9700
C6—C7	1.525 (6)	C36—C37	1.544 (4)
C6—H6A	0.9700	C37—C38	1.534 (5)
C6—H6B	0.9700	C37—H37	0.9800
C7—C21	1.532 (6)	C38—C39	1.526 (5)
C7—C22	1.538 (6)	C38—H38	0.95 (3)
C7—C8	1.584 (5)	C39—C40	1.546 (5)
C8—C9	1.499 (5)	C39—H39A	0.9700
C8—C12	1.546 (4)	C39—H39B	0.9700
C8—H8	0.95 (4)	C40—C41	1.494 (5)
C11—C12	1.527 (4)	C40—C43	1.521 (5)
C11—H11A	0.9700	C40—H40	0.95 (4)
C11—H11B	0.9700	C41—C44	1.317 (5)

C12—C13	1.553 (4)	C41—C42	1.484 (5)
C13—C14	1.532 (4)	C43—H43	0.98 (4)
C13—H13	0.9800	C44—H44A	0.9300
C14—C15	1.539 (4)	C44—H44B	0.9300
C14—H14	0.9800	C45—H45A	0.9600
C15—C16	1.544 (5)	C45—H45B	0.9600
C15—H15A	0.9700	C45—H45C	0.9600
C15—H15B	0.9700	C46—H46A	0.9600
C16—C17	1.495 (5)	C46—H46B	0.9600
C16—C19	1.519 (4)	C46—H46C	0.9600
C16—H16	0.9800	C47—C48	1.480 (6)
C17—C20	1.324 (5)	C48—H48A	0.9600
C17—C18	1.490 (5)	C48—H48B	0.9600
C19—H19	0.952 (18)	C48—H48C	0.9600
C2—O3—C4	118.1 (2)	H24A—C24—H24B	109.5
C14—O4—H4A	105 (3)	C23—C24—H24C	109.5
C23—O6—C19	118.0 (3)	H24A—C24—H24C	109.5
C9—O10—C11	109.6 (3)	H24B—C24—H24C	109.5
C26—O27—C28	117.3 (2)	C26—C25—C42	111.2 (3)
C38—O28—H28A	116 (3)	C26—C25—C43	112.7 (3)
C47—O30—C43	116.4 (3)	C42—C25—C43	101.1 (3)
C33—O34—C35	110.1 (2)	C26—C25—C37	116.6 (3)
C2—C1—C19	111.6 (2)	C42—C25—C37	104.2 (2)
C2—C1—C18	111.6 (3)	C43—C25—C37	109.6 (3)
C19—C1—C18	101.1 (3)	O25—C26—O27	118.6 (3)
C2—C1—C13	116.8 (2)	O25—C26—C25	122.0 (4)
C19—C1—C13	110.5 (2)	O27—C26—C25	119.4 (3)
C18—C1—C13	103.8 (2)	O27—C28—C29	109.4 (3)
O1—C2—O3	118.4 (3)	O27—C28—C36	107.8 (3)
O1—C2—C1	123.1 (3)	C29—C28—C36	113.5 (3)
O3—C2—C1	118.5 (3)	O27—C28—H28	107 (2)
O3—C4—C5	107.6 (3)	C29—C28—H28	111.5 (19)
O3—C4—C12	106.8 (2)	C36—C28—H28	107.6 (19)
C5—C4—C12	113.8 (3)	C28—C29—C30	108.7 (3)
O3—C4—H4	109.5	C28—C29—H29A	109.9
C5—C4—H4	109.5	C30—C29—H29A	109.9
C12—C4—H4	109.5	C28—C29—H29B	109.9
C4—C5—C6	108.1 (3)	C30—C29—H29B	109.9
C4—C5—H5A	110.1	H29A—C29—H29B	108.3
C6—C5—H5A	110.1	C29—C30—C31	112.8 (3)
C4—C5—H5B	110.1	C29—C30—H30A	109.0
C6—C5—H5B	110.1	C31—C30—H30A	109.0
H5A—C5—H5B	108.4	C29—C30—H30B	109.0
C5—C6—C7	113.4 (3)	C31—C30—H30B	109.0
C5—C6—H6A	108.9	H30A—C30—H30B	107.8
C7—C6—H6A	108.9	C46—C31—C30	110.2 (3)
C5—C6—H6B	108.9	C46—C31—C45	108.6 (3)
C7—C6—H6B	108.9	C30—C31—C45	108.7 (3)
H6A—C6—H6B	107.7	C46—C31—C32	113.8 (3)

C6—C7—C21	109.6 (4)	C30—C31—C32	107.8 (3)
C6—C7—C22	110.8 (3)	C45—C31—C32	107.6 (3)
C21—C7—C22	107.7 (3)	C33—C32—C36	102.4 (3)
C6—C7—C8	108.5 (3)	C33—C32—C31	108.9 (3)
C21—C7—C8	107.2 (3)	C36—C32—C31	117.4 (3)
C22—C7—C8	113.0 (3)	C33—C32—H32	111 (2)
C9—C8—C12	102.2 (3)	C36—C32—H32	114 (2)
C9—C8—C7	110.1 (3)	C31—C32—H32	103.2 (19)
C12—C8—C7	116.6 (3)	O26—C33—O34	120.5 (3)
C9—C8—H8	112 (2)	O26—C33—C32	128.8 (3)
C12—C8—H8	106 (2)	O34—C33—C32	110.7 (3)
C7—C8—H8	110 (2)	O34—C35—C36	105.9 (3)
O2—C9—O10	121.0 (4)	O34—C35—H35A	110.6
O2—C9—C8	128.5 (4)	C36—C35—H35A	110.6
O10—C9—C8	110.5 (3)	O34—C35—H35B	110.6
O10—C11—C12	106.3 (3)	C36—C35—H35B	110.6
O10—C11—H11A	110.5	H35A—C35—H35B	108.7
C12—C11—H11A	110.5	C28—C36—C35	111.8 (3)
O10—C11—H11B	110.5	C28—C36—C32	115.9 (3)
C12—C11—H11B	110.5	C35—C36—C32	100.7 (3)
H11A—C11—H11B	108.7	C28—C36—C37	107.3 (3)
C11—C12—C4	113.0 (3)	C35—C36—C37	107.7 (2)
C11—C12—C8	100.0 (3)	C32—C36—C37	113.2 (2)
C4—C12—C8	115.7 (3)	C38—C37—C36	115.6 (2)
C11—C12—C13	107.5 (2)	C38—C37—C25	112.0 (3)
C4—C12—C13	107.8 (2)	C36—C37—C25	110.3 (2)
C8—C12—C13	112.6 (2)	C38—C37—H37	106.1
C14—C13—C12	116.6 (2)	C36—C37—H37	106.1
C14—C13—C1	113.2 (2)	C25—C37—H37	106.1
C12—C13—C1	108.4 (2)	O28—C38—C39	110.8 (3)
C14—C13—H13	105.9	O28—C38—C37	109.3 (3)
C12—C13—H13	105.9	C39—C38—C37	111.7 (3)
C1—C13—H13	105.9	O28—C38—H38	104.1 (18)
O4—C14—C13	109.3 (2)	C39—C38—H38	110.8 (18)
O4—C14—C15	111.8 (3)	C37—C38—H38	109.9 (19)
C13—C14—C15	111.9 (3)	C38—C39—C40	113.1 (3)
O4—C14—H14	107.9	C38—C39—H39A	109.0
C13—C14—H14	107.9	C40—C39—H39A	109.0
C15—C14—H14	107.9	C38—C39—H39B	109.0
C14—C15—C16	114.0 (2)	C40—C39—H39B	109.0
C14—C15—H15A	108.7	H39A—C39—H39B	107.8
C16—C15—H15A	108.7	C41—C40—C43	102.1 (3)
C14—C15—H15B	108.7	C41—C40—C39	111.5 (3)
C16—C15—H15B	108.7	C43—C40—C39	108.4 (3)
H15A—C15—H15B	107.6	C41—C40—H40	113 (2)
C17—C16—C19	101.9 (3)	C43—C40—H40	109 (2)
C17—C16—C15	111.2 (3)	C39—C40—H40	112 (2)
C19—C16—C15	109.3 (3)	C44—C41—C42	122.4 (4)
C17—C16—H16	111.3	C44—C41—C40	128.9 (4)

C19—C16—H16	111.3	C42—C41—C40	108.7 (3)
C15—C16—H16	111.3	O29—C42—C41	128.6 (3)
C20—C17—C18	122.9 (4)	O29—C42—C25	126.0 (4)
C20—C17—C16	129.3 (4)	C41—C42—C25	105.3 (3)
C18—C17—C16	107.8 (3)	O30—C43—C40	107.4 (3)
O5—C18—C17	128.2 (3)	O30—C43—C25	109.3 (3)
O5—C18—C1	125.9 (3)	C40—C43—C25	101.5 (3)
C17—C18—C1	105.7 (3)	O30—C43—H43	112 (2)
O6—C19—C16	106.9 (3)	C40—C43—H43	116 (2)
O6—C19—C1	109.9 (3)	C25—C43—H43	111 (2)
C16—C19—C1	101.6 (2)	C41—C44—H44A	120.0
O6—C19—H19	112.0 (18)	C41—C44—H44B	120.0
C16—C19—H19	110.5 (17)	H44A—C44—H44B	120.0
C1—C19—H19	115.1 (18)	C31—C45—H45A	109.5
C17—C20—H20A	120.0	C31—C45—H45B	109.5
C17—C20—H20B	120.0	H45A—C45—H45B	109.5
H20A—C20—H20B	120.0	C31—C45—H45C	109.5
C7—C21—H21A	109.5	H45A—C45—H45C	109.5
C7—C21—H21B	109.5	H45B—C45—H45C	109.5
H21A—C21—H21B	109.5	C31—C46—H46A	109.5
C7—C21—H21C	109.5	C31—C46—H46B	109.5
H21A—C21—H21C	109.5	H46A—C46—H46B	109.5
H21B—C21—H21C	109.5	C31—C46—H46C	109.5
C7—C22—H22A	109.5	H46A—C46—H46C	109.5
C7—C22—H22B	109.5	H46B—C46—H46C	109.5
H22A—C22—H22B	109.5	O31—C47—O30	123.1 (4)
C7—C22—H22C	109.5	O31—C47—C48	126.2 (4)
H22A—C22—H22C	109.5	O30—C47—C48	110.6 (4)
H22B—C22—H22C	109.5	C47—C48—H48A	109.5
O7—C23—O6	123.2 (4)	C47—C48—H48B	109.5
O7—C23—C24	126.0 (4)	H48A—C48—H48B	109.5
O6—C23—C24	110.8 (4)	C47—C48—H48C	109.5
C23—C24—H24A	109.5	H48A—C48—H48C	109.5
C23—C24—H24B	109.5	H48B—C48—H48C	109.5
C4—O3—C2—O1	178.7 (3)	C28—O27—C26—O25	−176.7 (3)
C4—O3—C2—C1	−2.7 (4)	C28—O27—C26—C25	2.3 (4)
C19—C1—C2—O1	82.7 (4)	C42—C25—C26—O25	−33.7 (4)
C18—C1—C2—O1	−29.7 (4)	C43—C25—C26—O25	79.1 (4)
C13—C1—C2—O1	−148.8 (3)	C37—C25—C26—O25	−153.0 (3)
C19—C1—C2—O3	−95.8 (3)	C42—C25—C26—O27	147.3 (3)
C18—C1—C2—O3	151.8 (3)	C43—C25—C26—O27	−100.0 (3)
C13—C1—C2—O3	32.7 (4)	C37—C25—C26—O27	28.0 (4)
C2—O3—C4—C5	−172.3 (3)	C26—O27—C28—C29	−176.6 (3)
C2—O3—C4—C12	−49.7 (4)	C26—O27—C28—C36	−52.7 (4)
O3—C4—C5—C6	174.1 (3)	O27—C28—C29—C30	176.1 (3)
C12—C4—C5—C6	55.9 (4)	C36—C28—C29—C30	55.7 (4)
C4—C5—C6—C7	−66.5 (4)	C28—C29—C30—C31	−67.8 (4)
C5—C6—C7—C21	173.7 (3)	C29—C30—C31—C46	−67.3 (4)
C5—C6—C7—C22	−67.6 (4)	C29—C30—C31—C45	173.8 (3)

C5—C6—C7—C8	57.0 (4)	C29—C30—C31—C32	57.5 (4)
C6—C7—C8—C9	−155.1 (3)	C46—C31—C32—C33	−32.0 (4)
C21—C7—C8—C9	86.7 (4)	C30—C31—C32—C33	−154.5 (3)
C22—C7—C8—C9	−31.8 (4)	C45—C31—C32—C33	88.4 (4)
C6—C7—C8—C12	−39.3 (4)	C46—C31—C32—C36	83.7 (4)
C21—C7—C8—C12	−157.5 (3)	C30—C31—C32—C36	−38.9 (4)
C22—C7—C8—C12	84.0 (4)	C45—C31—C32—C36	−155.9 (3)
C11—O10—C9—O2	−178.0 (3)	C35—O34—C33—O26	179.9 (3)
C11—O10—C9—C8	1.9 (4)	C35—O34—C33—C32	1.7 (3)
C12—C8—C9—O2	157.8 (3)	C36—C32—C33—O26	161.1 (3)
C7—C8—C9—O2	−77.6 (4)	C31—C32—C33—O26	−73.9 (4)
C12—C8—C9—O10	−22.1 (3)	C36—C32—C33—O34	−20.9 (3)
C7—C8—C9—O10	102.5 (3)	C31—C32—C33—O34	104.1 (3)
C9—O10—C11—C12	19.7 (3)	C33—O34—C35—C36	18.6 (3)
O10—C11—C12—C4	−155.2 (2)	O27—C28—C36—C35	−45.8 (3)
O10—C11—C12—C8	−31.6 (3)	C29—C28—C36—C35	75.6 (4)
O10—C11—C12—C13	86.0 (3)	O27—C28—C36—C32	−160.4 (3)
O3—C4—C12—C11	−45.2 (3)	C29—C28—C36—C32	−39.1 (4)
C5—C4—C12—C11	73.4 (4)	O27—C28—C36—C37	72.1 (3)
O3—C4—C12—C8	−159.7 (3)	C29—C28—C36—C37	−166.6 (3)
C5—C4—C12—C8	−41.0 (4)	O34—C35—C36—C28	−153.6 (3)
O3—C4—C12—C13	73.4 (3)	O34—C35—C36—C32	−29.9 (3)
C5—C4—C12—C13	−168.0 (3)	O34—C35—C36—C37	88.8 (3)
C9—C8—C12—C11	31.3 (3)	C33—C32—C36—C28	150.4 (3)
C7—C8—C12—C11	−88.9 (3)	C31—C32—C36—C28	31.3 (4)
C9—C8—C12—C4	152.9 (3)	C33—C32—C36—C35	29.6 (3)
C7—C8—C12—C4	32.8 (4)	C31—C32—C36—C35	−89.5 (3)
C9—C8—C12—C13	−82.5 (3)	C33—C32—C36—C37	−85.0 (3)
C7—C8—C12—C13	157.3 (3)	C31—C32—C36—C37	155.8 (3)
C11—C12—C13—C14	−151.4 (3)	C28—C36—C37—C38	87.4 (3)
C4—C12—C13—C14	86.5 (3)	C35—C36—C37—C38	−152.1 (3)
C8—C12—C13—C14	−42.2 (4)	C32—C36—C37—C38	−41.7 (4)
C11—C12—C13—C1	79.4 (3)	C28—C36—C37—C25	−40.9 (3)
C4—C12—C13—C1	−42.6 (3)	C35—C36—C37—C25	79.6 (3)
C8—C12—C13—C1	−171.4 (3)	C32—C36—C37—C25	−170.0 (3)
C2—C1—C13—C14	−137.5 (3)	C26—C25—C37—C38	−135.5 (3)
C19—C1—C13—C14	−8.4 (3)	C42—C25—C37—C38	101.5 (3)
C18—C1—C13—C14	99.3 (3)	C43—C25—C37—C38	−6.1 (3)
C2—C1—C13—C12	−6.4 (3)	C26—C25—C37—C36	−5.3 (4)
C19—C1—C13—C12	122.6 (3)	C42—C25—C37—C36	−128.3 (3)
C18—C1—C13—C12	−129.7 (3)	C43—C25—C37—C36	124.1 (3)
C12—C13—C14—O4	−46.0 (4)	C36—C37—C38—O28	−52.3 (4)
C1—C13—C14—O4	80.9 (3)	C25—C37—C38—O28	75.1 (3)
C12—C13—C14—C15	−170.3 (2)	C36—C37—C38—C39	−175.2 (3)
C1—C13—C14—C15	−43.5 (3)	C25—C37—C38—C39	−47.8 (4)
O4—C14—C15—C16	−86.0 (3)	O28—C38—C39—C40	−81.6 (4)
C13—C14—C15—C16	37.0 (4)	C37—C38—C39—C40	40.5 (4)
C14—C15—C16—C17	−90.0 (3)	C38—C39—C40—C41	−90.6 (4)
C14—C15—C16—C19	21.8 (4)	C38—C39—C40—C43	21.0 (4)

C19—C16—C17—C20	152.3 (4)	C43—C40—C41—C44	155.4 (4)
C15—C16—C17—C20	−91.3 (4)	C39—C40—C41—C44	−89.1 (5)
C19—C16—C17—C18	−28.4 (3)	C43—C40—C41—C42	−26.6 (4)
C15—C16—C17—C18	88.1 (3)	C39—C40—C41—C42	88.9 (3)
C20—C17—C18—O5	4.3 (6)	C44—C41—C42—O29	0.5 (6)
C16—C17—C18—O5	−175.1 (3)	C40—C41—C42—O29	−177.6 (4)
C20—C17—C18—C1	−179.7 (3)	C44—C41—C42—C25	177.1 (4)
C16—C17—C18—C1	0.9 (3)	C40—C41—C42—C25	−1.0 (4)
C2—C1—C18—O5	−38.6 (4)	C26—C25—C42—O29	−35.7 (5)
C19—C1—C18—O5	−157.4 (3)	C43—C25—C42—O29	−155.6 (4)
C13—C1—C18—O5	88.0 (4)	C37—C25—C42—O29	90.7 (4)
C2—C1—C18—C17	145.3 (3)	C26—C25—C42—C41	147.6 (3)
C19—C1—C18—C17	26.5 (3)	C43—C25—C42—C41	27.7 (3)
C13—C1—C18—C17	−88.1 (3)	C37—C25—C42—C41	−86.0 (3)
C23—O6—C19—C16	−153.8 (3)	C47—O30—C43—C40	−153.7 (3)
C23—O6—C19—C1	96.7 (3)	C47—O30—C43—C25	97.0 (3)
C17—C16—C19—O6	−70.5 (3)	C41—C40—C43—O30	−71.2 (3)
C15—C16—C19—O6	171.7 (3)	C39—C40—C43—O30	171.1 (3)
C17—C16—C19—C1	44.7 (3)	C41—C40—C43—C25	43.4 (3)
C15—C16—C19—C1	−73.1 (3)	C39—C40—C43—C25	−74.3 (3)
C2—C1—C19—O6	−49.6 (3)	C26—C25—C43—O30	−49.4 (3)
C18—C1—C19—O6	69.2 (3)	C42—C25—C43—O30	69.4 (3)
C13—C1—C19—O6	178.6 (2)	C37—C25—C43—O30	179.0 (2)
C2—C1—C19—C16	−162.6 (3)	C26—C25—C43—C40	−162.6 (3)
C18—C1—C19—C16	−43.8 (3)	C42—C25—C43—C40	−43.8 (3)
C13—C1—C19—C16	65.7 (3)	C37—C25—C43—C40	65.8 (3)
C19—O6—C23—O7	1.1 (5)	C43—O30—C47—O31	1.2 (6)
C19—O6—C23—C24	−178.7 (3)	C43—O30—C47—C48	−176.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O28—H28A···O1^{i}	0.81 (2)	1.93 (2)	2.711 (3)	161 (4)
O4—H4A···O26	0.84 (2)	2.20 (3)	2.957 (4)	150 (4)

Symmetry codes: (i) *x*+1, *y*, *z*.

Fig. 1

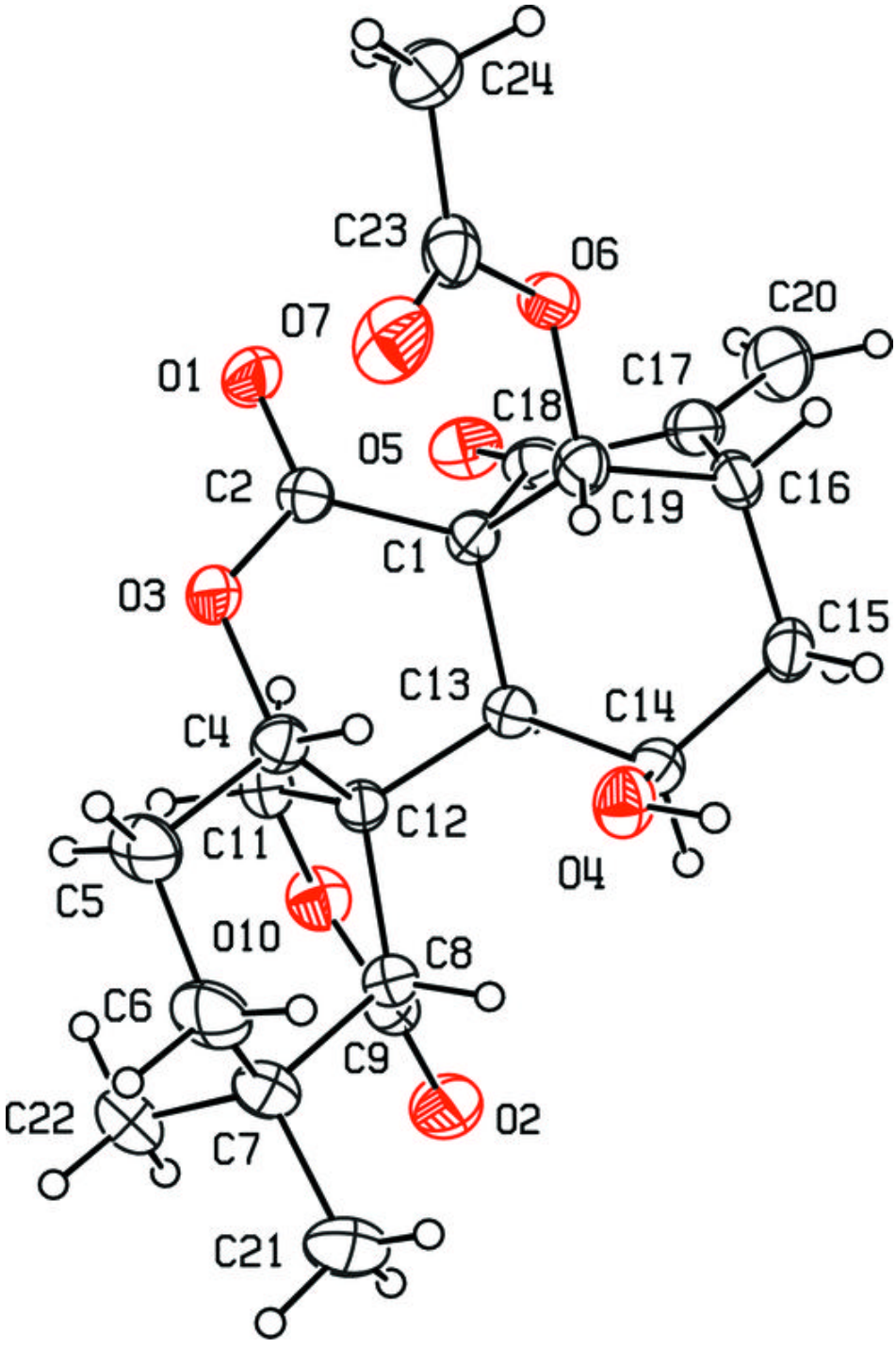
C24
C23
O6
O7
C20
O1
C17
C18
O5
C2
C19
C16
C1
O3
C15
C13
C14
C4
C12
C11
O4
C5
O10
C8
C6
C9
O2
C22
C7
C21

Fig. 2

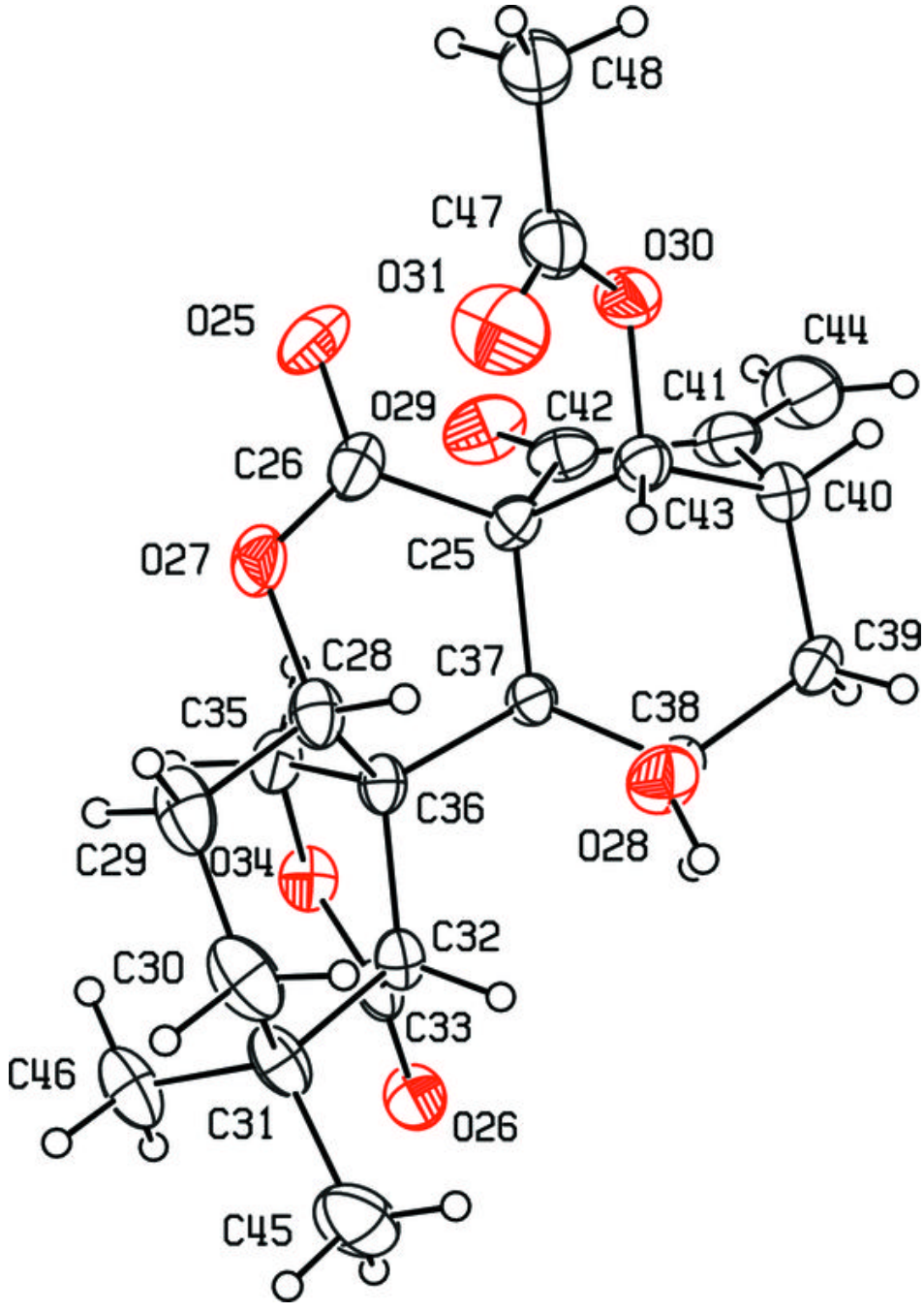
C48
C47
O30
O31
O25
C44
C41
O29
C42
C26
C40
C43
O27
C25
C39
C28
C37
C35
C38
C36
C29
O34
O28
C32
C30
C33
C46
O26
C31
C45

Fig. 3