Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Euphorbia Factor L_2: an ester of 7-hydroxylathyrol

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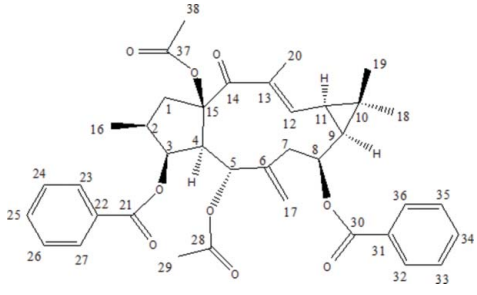
Received 2 November 2007; accepted 5 November 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.010 Å; R factor = 0.054; wR factor = 0.171; data-to-parameter ratio = 8.6.

In the crystal structure of the title macrocyclic diterpenoid [systematic name: (2*S**,3*S**,4*R**,5*R**,7*R**,9*S**,11*S**,15*R**)-5,15-diacetoxy-14-oxolathyra-6(17),12(*E*)-diene-3,7-diyl dibenzoate], $C_{38}H_{42}O_9$, the molecule exhibits the tricyclic terpenoid skeleton of lathyrane, consisting of fused five-, 11- and three-membered rings. The five-membered ring adopts an envelope conformation. Intra- and intermolecular weak C—H···O hydrogen bonding helps to stabilize the crystal structure.

Related literature

For general background, see: Bicchi, *et al.* (2001); For a related structure, see: Appendino *et al.* (1999).



Experimental

Crystal data

$C_{38}H_{42}O_9$
M_r = 642.72
Orthorhombic, $P2_12_12_1$
a = 13.418 (6) Å
b = 14.989 (4) Å
c = 18.126 (5) Å
V = 3646 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.36 × 0.34 × 0.25 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
3800 measured reflections
3765 independent reflections
1525 reflections with $I > 2\sigma(I)$
R_{int} = 0.006
3 standard reflections
every 300 reflections
intensity decay: 1.2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.171
S = 0.91
3765 reflections
436 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 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
C12—H12···O3	0.93	2.23	2.946 (8)	134
C17—H17B···O9^{i}	0.93	2.39	3.222 (9)	150
C19—H19A···O1^{ii}	0.96	2.54	3.427 (10)	153
C35—H35···O5^{ii}	0.93	2.58	3.218 (9)	126

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

Data collection: *DIFRAC* (Gabe & White, 1993); cell refinement: *DIFRAC* ; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Support by the Western Light Joint Research Program from the Chinese Academy of Sciences is acknowledged. We are also grateful to the staff of the analytical group of Chengdu Institute of Biology, Chinese Academy of Sciences, for measuring the NMR spectra.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2355).

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 doi:10.1107/S1600536807055900

supplementary materials

Acta Cryst. (2007). E**63**, o4613 [**doi:10.1107/S1600536807055900**]

Euphorbia Factor L_2: an ester of 7-hydroxylathyrol

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Comment

Euphorbia is the genus in the family Euphorbiaceae, and is widely distributed throughout the world. Many species of this genus are being used as traditional drugs in China such as *Euphorbia Fischeriana* Steud. and *Euphorbia kansui L.*. Plants belonging to *Euphorbia* are known to be rich sources of terpenoids, especially various diterpenoids. Previous chemical investigations on the seeds of *Euphorbia lathyris* were focused on lathyrol and ingenol diterpenoids (Bicchi, *et al.* 2001). As a part of our research on the chemical constituents from this medicine, the title compound was isolated. Its structure was elucidated by spectroscopic analysis and was confirmed by single-crystal X-ray diffraction analysis.

The title compound shows the tricyclic terpenoid skeleton of lathyrane (Fig. 1), consisting of fused five-, eleven- and three-membered rings (A: C1–C4/C15, B: C4–C9/C11–C15, C: C9–C11). Rings A and B are *trans*-joined (H4–C4–C15–O3 = −153.7°), while rings B and C are *cis*-joined (H9–C9–C11–H11 = 1.13°). Ring A adopts an envelope conformation, with atom C3 0.65 Å out of the plane defined by atoms C1/C2/C4/C15. Intra-molecular and inter-molecular weak C—H···O hydrogen bonding helps to stabilize the crystal structure (Table 1).

Experimental

The seeds of *Euphorbia lathyris* were collected in Sichuan province of China. The powdered seeds (10 kg) were extracted with EtOH three times and filtered. The filtrate was evaporated *in vacuo*, the residue was suspended in H_2O and partitioned successively with EtOA. This EtOA extract was subjected to column chromatography on Si gel eluted with petroleum-EtOA (15:1, 10:1, 8:1, 4:1, 2:1 and 1:1) and methanol to yield fractions 1–10. Fraction 3 (10 g) was chromatographed over Si gel (petroleum ether-EtOA, 4:1) to give three fractions. The second fraction was eluted with petroleum-acetone (5:1) on Si gel, followed by RP18 (MeOH-H_2O, 85:15) to provide the pure title compound as colorless crystals. Suitable crystals were obtained by slow evaporation of a methanol solution at room temperature.

Refinement

All hydrogen atoms were located geometrically with C—H distances of 0.93–0.98 Å, and refined using a riding model. The absolute configuration could not be determined from the X-ray analysis, owing to the absence of significant anomalous scatterers, and Friedel pairs were averaged. The current absolute configuration was assigned by reference to the chiral molecule of known absolute configuration which had been confirmed on a biogenetic basis (Appendino, *et al.*, 1999).

Figures

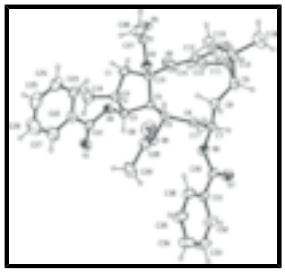

Fig. 1. View of the molecule of (I) showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

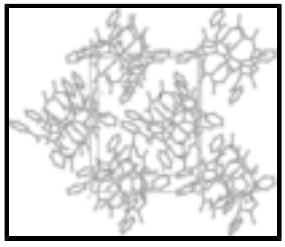

Fig. 2. The crystal packing of (I), viewed down the A axis. H-atoms were omitted for clarity.

(I)

Crystal data

$C_{38}H_{42}O_9$	F_{000} = 1368
M_r = 642.72	D_x = 1.171 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 27 reflections
a = 13.418 (6) Å	θ = 4.5–5.7º
b = 14.989 (4) Å	μ = 0.08 mm^{-1}
c = 18.126 (5) Å	T = 298 (2) K
V = 3646 (2) Å^3	Block, colourless
Z = 4	0.36 × 0.34 × 0.25 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.006
Radiation source: fine-focus sealed tube	θ_{max} = 25.5º
Monochromator: graphite	θ_{min} = 1.8º
T = 298(2) K	h = −1→16
ω/2–θ scans	k = −3→18
Absorption correction: none	l = −2→21
3800 measured reflections	3 standard reflections
3765 independent reflections	every 300 reflections
1525 reflections with $I > 2\sigma(I)$	intensity decay: 1.2%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.054$

$wR(F^2) = 0.171$

$S = 0.91$

3765 reflections

436 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.092P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.18$ e Å^{-3}

$\Delta\rho_{min} = -0.17$ e Å^{-3}

Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0043 (9)

Special details

Experimental. ^{13}C NMR (150 MHz, $CDCl_3$, δ, p.p.m.): 47.88(C1), 37.63(C2), 79.55(C3), 52.92(C4), 64.24(C5), 142.09 (C6), 78.57(C7), 28.79(C8), 31.54(C9), 24.65(C10), 27.78(C11), 142.61 (C12), 135.56(C13), 197.53(C14), 91.98 (C15), 14.12(C16), 119.60(C17), 28.68(C18), 16.61(C19), 12.73(C20), 165.97(C21), 130.34(C22),129.65(C23), 128.31(C24), 135.56(C25), 128.31(C26), 129.65(C27), 169.69(C28), 21.83(C29), 165.60(C30), 130.16(C31), 129.60(C32), 128.32(C33), 135.56(C34), 128.32(C35), 129.60(C36), 169.33(C37), 20.91(C38).

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	1.0377 (5)	0.2624 (4)	0.7591 (3)	0.122 (2)
O2	0.9735 (3)	0.3457 (3)	0.8502 (2)	0.0665 (12)
O3	0.9039 (3)	0.4391 (2)	0.9900 (2)	0.0678 (12)
O4	0.9028 (5)	0.5847 (3)	1.0151 (4)	0.124 (2)
O5	1.1394 (4)	0.5087 (4)	1.0605 (3)	0.114 (2)
O6	0.9231 (3)	0.0905 (2)	1.0792 (2)	0.0647 (12)
O7	1.0540 (4)	0.0179 (3)	1.1286 (3)	0.0835 (14)
O8	0.9920 (3)	0.1948 (2)	0.9494 (2)	0.0651 (12)
O9	0.8264 (4)	0.1850 (4)	0.9472 (4)	0.108 (2)

C1	1.0492 (6)	0.4971 (4)	0.9242 (4)	0.083 (2)
H1A	0.9928	0.5168	0.8949	0.066 (9)*
H1B	1.0856	0.5491	0.9410	0.066 (9)*
C2	1.1172 (5)	0.4361 (4)	0.8783 (4)	0.074 (2)
H2	1.1830	0.4345	0.9016	0.074 (7)*
C3	1.0681 (5)	0.3479 (4)	0.8898 (3)	0.0649 (18)
H3	1.1117	0.2991	0.8740	0.074 (7)*
C4	1.0490 (4)	0.3439 (3)	0.9722 (3)	0.0511 (15)
H4	1.1150	0.3385	0.9948	0.074 (7)*
C5	0.9883 (4)	0.2666 (3)	1.0035 (3)	0.0490 (15)
H5	0.9189	0.2861	1.0084	0.074 (7)*
C6	1.0215 (5)	0.2276 (4)	1.0770 (3)	0.0541 (15)
C7	0.9500 (5)	0.1715 (3)	1.1211 (3)	0.0543 (16)
H7	0.9843	0.1526	1.1663	0.074 (7)*
C8	0.8521 (5)	0.2145 (4)	1.1434 (3)	0.0622 (17)
H8A	0.8298	0.2522	1.1032	0.066 (9)*
H8B	0.8028	0.1678	1.1497	0.066 (9)*
C9	0.8550 (5)	0.2695 (5)	1.2126 (3)	0.0660 (19)
H9	0.8699	0.2341	1.2567	0.074 (7)*
C10	0.7880 (5)	0.3469 (5)	1.2283 (4)	0.0680 (19)
C11	0.9000 (5)	0.3631 (4)	1.2156 (3)	0.0696 (19)
H11	0.9391	0.3768	1.2599	0.074 (7)*
C12	0.9366 (5)	0.4015 (4)	1.1477 (4)	0.0618 (17)
H12	0.9004	0.3881	1.1054	0.118 (9)*
C13	1.0172 (5)	0.4546 (4)	1.1383 (4)	0.0719 (19)
C14	1.0577 (5)	0.4734 (4)	1.0657 (4)	0.0721 (19)
C15	1.0136 (5)	0.4413 (4)	0.9903 (4)	0.0613 (18)
C16	1.1299 (6)	0.4676 (6)	0.7974 (4)	0.106 (3)
H16A	1.0657	0.4811	0.7768	0.143 (8)*
H16B	1.1608	0.4211	0.7691	0.143 (8)*
H16C	1.1710	0.5199	0.7962	0.143 (8)*
C17	1.1122 (5)	0.2392 (5)	1.1031 (4)	0.086 (2)
H17A	1.1305	0.2131	1.1476	0.12 (2)*
H17B	1.1579	0.2736	1.0770	0.12 (2)*
C18	0.7534 (6)	0.3568 (6)	1.3075 (4)	0.105 (3)
H18A	0.6909	0.3266	1.3137	0.143 (8)*
H18B	0.7452	0.4189	1.3188	0.143 (8)*
H18C	0.8021	0.3312	1.3400	0.143 (8)*
C19	0.7140 (5)	0.3800 (5)	1.1713 (4)	0.085 (2)
H19A	0.6511	0.3507	1.1785	0.143 (8)*
H19B	0.7385	0.3671	1.1227	0.143 (8)*
H19C	0.7055	0.4433	1.1766	0.143 (8)*
C20	1.0775 (6)	0.4896 (7)	1.2024 (4)	0.126 (4)
H20A	1.1420	0.4617	1.2025	0.143 (8)*
H20B	1.0437	0.4762	1.2478	0.143 (8)*
H20C	1.0853	0.5530	1.1977	0.143 (8)*
C21	0.9704 (6)	0.3046 (5)	0.7848 (4)	0.082 (2)
C22	0.8711 (6)	0.3159 (5)	0.7483 (4)	0.081 (2)
C23	0.8010 (6)	0.3731 (5)	0.7735 (4)	0.075 (2)

H23	0.8130	0.4059	0.8162	0.118 (9)*
C24	0.7110 (7)	0.3833 (6)	0.7363 (6)	0.097 (3)
H24	0.6632	0.4223	0.7547	0.118 (9)*
C25	0.6925 (8)	0.3379 (8)	0.6745 (6)	0.128 (4)
H25	0.6323	0.3456	0.6499	0.118 (9)*
C26	0.7630 (10)	0.2791 (9)	0.6470 (6)	0.183 (6)
H26	0.7503	0.2470	0.6041	0.118 (9)*
C27	0.8542 (8)	0.2686 (8)	0.6849 (5)	0.153 (5)
H27	0.9024	0.2297	0.6669	0.118 (9)*
C28	0.9038 (7)	0.1608 (5)	0.9250 (4)	0.080 (2)
C29	0.9208 (7)	0.0912 (6)	0.8680 (4)	0.123 (3)
H29A	0.9411	0.1189	0.8227	0.143 (8)*
H29B	0.8602	0.0585	0.8601	0.143 (8)*
H29C	0.9720	0.0511	0.8845	0.143 (8)*
C30	0.9808 (6)	0.0189 (4)	1.0890 (4)	0.0637 (17)
C31	0.9457 (5)	−0.0591 (4)	1.0448 (3)	0.0580 (16)
C32	1.0046 (5)	−0.1350 (4)	1.0458 (4)	0.082 (2)
H32	1.0637	−0.1356	1.0726	0.118 (9)*
C33	0.9758 (7)	−0.2095 (5)	1.0072 (5)	0.105 (3)
H33	1.0148	−0.2607	1.0085	0.118 (9)*
C34	0.8890 (6)	−0.2084 (5)	0.9664 (5)	0.104 (3)
H34	0.8708	−0.2579	0.9386	0.118 (9)*
C35	0.8301 (6)	−0.1345 (4)	0.9672 (5)	0.094 (3)
H35	0.7704	−0.1345	0.9412	0.118 (9)*
C36	0.8580 (5)	−0.0600 (4)	1.0059 (4)	0.075 (2)
H36	0.8172	−0.0098	1.0058	0.118 (9)*
C37	0.8580 (7)	0.5183 (6)	1.0018 (4)	0.086 (2)
C38	0.7478 (6)	0.5077 (6)	0.9931 (5)	0.116 (3)
H38A	0.7319	0.5012	0.9417	0.143 (8)*
H38B	0.7146	0.5594	1.0124	0.143 (8)*
H38C	0.7261	0.4557	1.0194	0.143 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.132 (5)	0.157 (5)	0.076 (3)	0.091 (5)	−0.009 (4)	−0.026 (4)
O2	0.061 (3)	0.080 (3)	0.058 (3)	0.030 (2)	0.003 (2)	−0.006 (2)
O3	0.074 (3)	0.052 (2)	0.078 (3)	0.017 (2)	0.012 (3)	0.002 (2)
O4	0.165 (6)	0.045 (3)	0.163 (6)	0.014 (4)	0.063 (5)	0.003 (3)
O5	0.087 (4)	0.128 (4)	0.128 (4)	−0.074 (4)	0.042 (3)	−0.038 (4)
O6	0.065 (3)	0.046 (2)	0.083 (3)	−0.010 (2)	−0.021 (3)	0.001 (2)
O7	0.069 (3)	0.080 (3)	0.102 (4)	0.010 (3)	−0.025 (3)	−0.007 (3)
O8	0.072 (3)	0.056 (2)	0.067 (3)	−0.007 (2)	−0.004 (2)	−0.014 (2)
O9	0.066 (3)	0.115 (4)	0.142 (5)	−0.005 (3)	−0.036 (4)	−0.002 (4)
C1	0.096 (5)	0.049 (4)	0.105 (5)	0.005 (4)	0.020 (5)	0.008 (4)
C2	0.067 (5)	0.069 (4)	0.087 (5)	0.008 (4)	0.023 (4)	0.015 (4)
C3	0.055 (4)	0.067 (4)	0.073 (5)	0.018 (4)	0.012 (4)	0.004 (4)
C4	0.046 (3)	0.046 (3)	0.061 (4)	0.004 (3)	0.004 (3)	0.002 (3)

C5	0.045 (3)	0.044 (3)	0.058 (4)	0.000 (3)	0.005 (3)	−0.008 (3)
C6	0.056 (4)	0.046 (3)	0.061 (4)	−0.002 (3)	−0.009 (3)	0.005 (3)
C7	0.062 (4)	0.048 (3)	0.052 (3)	−0.003 (3)	−0.009 (3)	0.004 (3)
C8	0.059 (4)	0.059 (4)	0.069 (4)	−0.015 (3)	−0.001 (3)	0.006 (4)
C9	0.057 (4)	0.086 (5)	0.055 (4)	−0.024 (4)	0.003 (3)	0.010 (4)
C10	0.063 (4)	0.081 (5)	0.060 (4)	−0.026 (4)	0.018 (4)	−0.012 (4)
C11	0.069 (5)	0.086 (5)	0.054 (4)	−0.032 (4)	−0.001 (4)	−0.009 (4)
C12	0.055 (4)	0.058 (4)	0.072 (4)	−0.018 (3)	0.013 (4)	−0.011 (3)
C13	0.067 (4)	0.077 (4)	0.072 (5)	−0.018 (4)	0.007 (4)	−0.025 (4)
C14	0.075 (5)	0.050 (3)	0.091 (5)	−0.023 (4)	0.031 (4)	−0.024 (4)
C15	0.050 (4)	0.051 (3)	0.082 (5)	−0.004 (3)	0.025 (4)	0.012 (3)
C16	0.112 (7)	0.119 (7)	0.087 (5)	0.015 (6)	0.042 (5)	0.032 (5)
C17	0.057 (4)	0.094 (5)	0.107 (6)	−0.011 (4)	−0.015 (4)	0.037 (5)
C18	0.093 (6)	0.127 (7)	0.095 (6)	−0.057 (5)	0.027 (5)	−0.018 (5)
C19	0.077 (5)	0.090 (5)	0.089 (5)	−0.017 (5)	0.009 (5)	−0.020 (4)
C20	0.096 (6)	0.183 (9)	0.099 (6)	−0.080 (7)	0.016 (5)	−0.053 (6)
C21	0.078 (5)	0.094 (5)	0.072 (5)	0.041 (5)	0.001 (4)	0.014 (4)
C22	0.100 (6)	0.086 (5)	0.058 (5)	0.009 (5)	0.001 (4)	0.004 (4)
C23	0.066 (5)	0.081 (5)	0.078 (5)	0.008 (4)	0.009 (4)	0.018 (4)
C24	0.075 (6)	0.108 (6)	0.107 (7)	0.007 (5)	0.008 (6)	0.037 (6)
C25	0.105 (8)	0.175 (11)	0.103 (8)	0.009 (8)	−0.029 (7)	0.033 (8)
C26	0.167 (12)	0.256 (15)	0.126 (9)	0.086 (12)	−0.072 (9)	−0.065 (10)
C27	0.157 (10)	0.196 (11)	0.105 (7)	0.092 (9)	−0.041 (7)	−0.049 (8)
C28	0.101 (6)	0.078 (5)	0.061 (5)	−0.026 (5)	−0.030 (5)	−0.006 (4)
C29	0.162 (9)	0.127 (7)	0.080 (5)	−0.042 (7)	−0.010 (6)	−0.036 (5)
C30	0.062 (4)	0.056 (4)	0.073 (4)	−0.004 (4)	0.000 (4)	0.016 (4)
C31	0.048 (4)	0.048 (3)	0.078 (4)	−0.002 (3)	−0.002 (4)	0.005 (3)
C32	0.055 (4)	0.068 (4)	0.122 (6)	−0.003 (4)	−0.014 (4)	0.000 (4)
C33	0.093 (6)	0.055 (4)	0.166 (8)	0.019 (5)	−0.022 (6)	−0.011 (5)
C34	0.082 (6)	0.068 (5)	0.161 (8)	0.000 (5)	−0.030 (6)	−0.038 (5)
C35	0.083 (6)	0.058 (4)	0.140 (7)	0.005 (4)	−0.042 (5)	−0.015 (5)
C36	0.066 (5)	0.061 (4)	0.096 (5)	0.009 (4)	−0.019 (4)	0.003 (4)
C37	0.107 (7)	0.065 (5)	0.088 (5)	0.039 (5)	0.029 (5)	0.021 (5)
C38	0.096 (7)	0.132 (7)	0.120 (7)	0.062 (6)	0.019 (5)	0.022 (6)

Geometric parameters (Å, °)

O1—C21	1.198 (8)	C16—H16A	0.9600
O2—C21	1.337 (8)	C16—H16B	0.9600
O2—C3	1.458 (7)	C16—H16C	0.9600
O3—C37	1.355 (8)	C17—H17A	0.9300
O3—C15	1.472 (7)	C17—H17B	0.9300
O4—C37	1.187 (9)	C18—H18A	0.9600
O5—C14	1.222 (7)	C18—H18B	0.9600
O6—C30	1.336 (7)	C18—H18C	0.9600
O6—C7	1.477 (6)	C19—H19A	0.9600
O7—C30	1.216 (7)	C19—H19B	0.9600
O8—C28	1.363 (8)	C19—H19C	0.9600
O8—C5	1.456 (6)	C20—H20A	0.9600

O9—C28	1.171 (9)	C20—H20B	0.9600
C1—C2	1.536 (8)	C20—H20C	0.9600
C1—C15	1.537 (8)	C21—C22	1.498 (10)
C1—H1A	0.9700	C22—C23	1.353 (9)
C1—H1B	0.9700	C22—C27	1.369 (11)
C2—C3	1.491 (8)	C23—C24	1.391 (10)
C2—C16	1.549 (8)	C23—H23	0.9300
C2—H2	0.9800	C24—C25	1.333 (12)
C3—C4	1.517 (7)	C24—H24	0.9300
C3—H3	0.9800	C25—C26	1.385 (13)
C4—C5	1.527 (7)	C25—H25	0.9300
C4—C15	1.570 (8)	C26—C27	1.412 (14)
C4—H4	0.9800	C26—H26	0.9300
C5—C6	1.520 (8)	C27—H27	0.9300
C5—H5	0.9800	C28—C29	1.486 (10)
C6—C17	1.317 (8)	C29—H29A	0.9600
C6—C7	1.507 (8)	C29—H29B	0.9600
C7—C8	1.518 (8)	C29—H29C	0.9600
C7—H7	0.9800	C30—C31	1.493 (8)
C8—C9	1.503 (8)	C31—C36	1.371 (9)
C8—H8A	0.9700	C31—C32	1.386 (8)
C8—H8B	0.9700	C32—C33	1.373 (9)
C9—C10	1.495 (10)	C32—H32	0.9300
C9—C11	1.528 (9)	C33—C34	1.379 (11)
C9—H9	0.9800	C33—H33	0.9300
C10—C19	1.516 (10)	C34—C35	1.361 (9)
C10—C18	1.516 (9)	C34—H34	0.9300
C10—C11	1.540 (9)	C35—C36	1.370 (9)
C11—C12	1.445 (8)	C35—H35	0.9300
C11—H11	0.9800	C36—H36	0.9300
C12—C13	1.354 (8)	C37—C38	1.495 (12)
C12—H12	0.9300	C38—H38A	0.9600
C13—C14	1.451 (9)	C38—H38B	0.9600
C13—C20	1.510 (9)	C38—H38C	0.9600
C14—C15	1.566 (9)		

C21—O2—C3	118.3 (5)	C2—C16—H16C	109.5
C37—O3—C15	115.7 (6)	H16A—C16—H16C	109.5
C30—O6—C7	116.8 (5)	H16B—C16—H16C	109.5
C28—O8—C5	117.7 (5)	C6—C17—H17A	120.0
C2—C1—C15	106.5 (5)	C6—C17—H17B	120.0
C2—C1—H1A	110.4	H17A—C17—H17B	120.0
C15—C1—H1A	110.4	C10—C18—H18A	109.5
C2—C1—H1B	110.4	C10—C18—H18B	109.5
C15—C1—H1B	110.4	H18A—C18—H18B	109.5
H1A—C1—H1B	108.6	C10—C18—H18C	109.5
C3—C2—C1	100.9 (5)	H18A—C18—H18C	109.5
C3—C2—C16	116.8 (6)	H18B—C18—H18C	109.5
C1—C2—C16	113.4 (6)	C10—C19—H19A	109.5
C3—C2—H2	108.4	C10—C19—H19B	109.5

C1—C2—H2	108.4	H19A—C19—H19B	109.5
C16—C2—H2	108.4	C10—C19—H19C	109.5
O2—C3—C2	109.6 (5)	H19A—C19—H19C	109.5
O2—C3—C4	109.7 (5)	H19B—C19—H19C	109.5
C2—C3—C4	104.3 (5)	C13—C20—H20A	109.5
O2—C3—H3	111.0	C13—C20—H20B	109.5
C2—C3—H3	111.0	H20A—C20—H20B	109.5
C4—C3—H3	111.0	C13—C20—H20C	109.5
C3—C4—C5	119.2 (5)	H20A—C20—H20C	109.5
C3—C4—C15	102.7 (5)	H20B—C20—H20C	109.5
C5—C4—C15	117.8 (4)	O1—C21—O2	124.4 (7)
C3—C4—H4	105.3	O1—C21—C22	124.0 (7)
C5—C4—H4	105.3	O2—C21—C22	111.6 (6)
C15—C4—H4	105.3	C23—C22—C27	119.8 (8)
O8—C5—C6	107.2 (4)	C23—C22—C21	122.7 (7)
O8—C5—C4	106.9 (4)	C27—C22—C21	117.4 (8)
C6—C5—C4	117.5 (5)	C22—C23—C24	120.5 (8)
O8—C5—H5	108.3	C22—C23—H23	119.7
C6—C5—H5	108.3	C24—C23—H23	119.7
C4—C5—H5	108.3	C25—C24—C23	120.9 (9)
C17—C6—C7	118.1 (6)	C25—C24—H24	119.6
C17—C6—C5	122.3 (6)	C23—C24—H24	119.6
C7—C6—C5	119.5 (5)	C24—C25—C26	120.0 (10)
O6—C7—C6	110.0 (5)	C24—C25—H25	120.0
O6—C7—C8	105.9 (5)	C26—C25—H25	120.0
C6—C7—C8	117.1 (4)	C25—C26—C27	119.2 (10)
O6—C7—H7	107.9	C25—C26—H26	120.4
C6—C7—H7	107.9	C27—C26—H26	120.4
C8—C7—H7	107.9	C22—C27—C26	119.6 (9)
C9—C8—C7	115.7 (5)	C22—C27—H27	120.2
C9—C8—H8A	108.4	C26—C27—H27	120.2
C7—C8—H8A	108.4	O9—C28—O8	122.8 (7)
C9—C8—H8B	108.4	O9—C28—C29	126.3 (8)
C7—C8—H8B	108.4	O8—C28—C29	110.8 (8)
H8A—C8—H8B	107.4	C28—C29—H29A	109.5
C10—C9—C8	124.7 (6)	C28—C29—H29B	109.5
C10—C9—C11	61.3 (4)	H29A—C29—H29B	109.5
C8—C9—C11	122.9 (5)	C28—C29—H29C	109.5
C10—C9—H9	112.9	H29A—C29—H29C	109.5
C8—C9—H9	112.9	H29B—C29—H29C	109.5
C11—C9—H9	112.9	O7—C30—O6	123.8 (6)
C9—C10—C19	121.3 (6)	O7—C30—C31	124.2 (6)
C9—C10—C18	116.1 (7)	O6—C30—C31	112.0 (6)
C19—C10—C18	114.3 (7)	C36—C31—C32	119.2 (6)
C9—C10—C11	60.4 (4)	C36—C31—C30	123.7 (6)
C19—C10—C11	119.1 (6)	C32—C31—C30	117.1 (6)
C18—C10—C11	115.1 (6)	C33—C32—C31	120.0 (7)
C12—C11—C9	118.0 (5)	C33—C32—H32	120.0
C12—C11—C10	121.4 (6)	C31—C32—H32	120.0

C9—C11—C10	58.3 (4)	C32—C33—C34	120.1 (7)
C12—C11—H11	115.6	C32—C33—H33	120.0
C9—C11—H11	115.6	C34—C33—H33	120.0
C10—C11—H11	115.6	C35—C34—C33	119.6 (7)
C13—C12—C11	127.8 (6)	C35—C34—H34	120.2
C13—C12—H12	116.1	C33—C34—H34	120.2
C11—C12—H12	116.1	C34—C35—C36	120.7 (7)
C12—C13—C14	121.8 (6)	C34—C35—H35	119.6
C12—C13—C20	122.4 (6)	C36—C35—H35	119.6
C14—C13—C20	115.4 (6)	C35—C36—C31	120.3 (6)
O5—C14—C13	119.4 (7)	C35—C36—H36	119.8
O5—C14—C15	113.9 (6)	C31—C36—H36	119.8
C13—C14—C15	126.2 (5)	O4—C37—O3	122.4 (8)
O3—C15—C1	108.7 (5)	O4—C37—C38	127.7 (8)
O3—C15—C14	112.8 (5)	O3—C37—C38	109.9 (8)
C1—C15—C14	113.4 (5)	C37—C38—H38A	109.5
O3—C15—C4	106.3 (5)	C37—C38—H38B	109.5
C1—C15—C4	104.4 (5)	H38A—C38—H38B	109.5
C14—C15—C4	110.7 (5)	C37—C38—H38C	109.5
C2—C16—H16A	109.5	H38A—C38—H38C	109.5
C2—C16—H16B	109.5	H38B—C38—H38C	109.5
H16A—C16—H16B	109.5		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O3	0.93	2.23	2.946 (8)	134
C17—H17B···O9^{i}	0.93	2.39	3.222 (9)	150
C19—H19A···O1^{ii}	0.96	2.54	3.427 (10)	153
C35—H35···O5^{ii}	0.93	2.58	3.218 (9)	126

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

Fig. 1

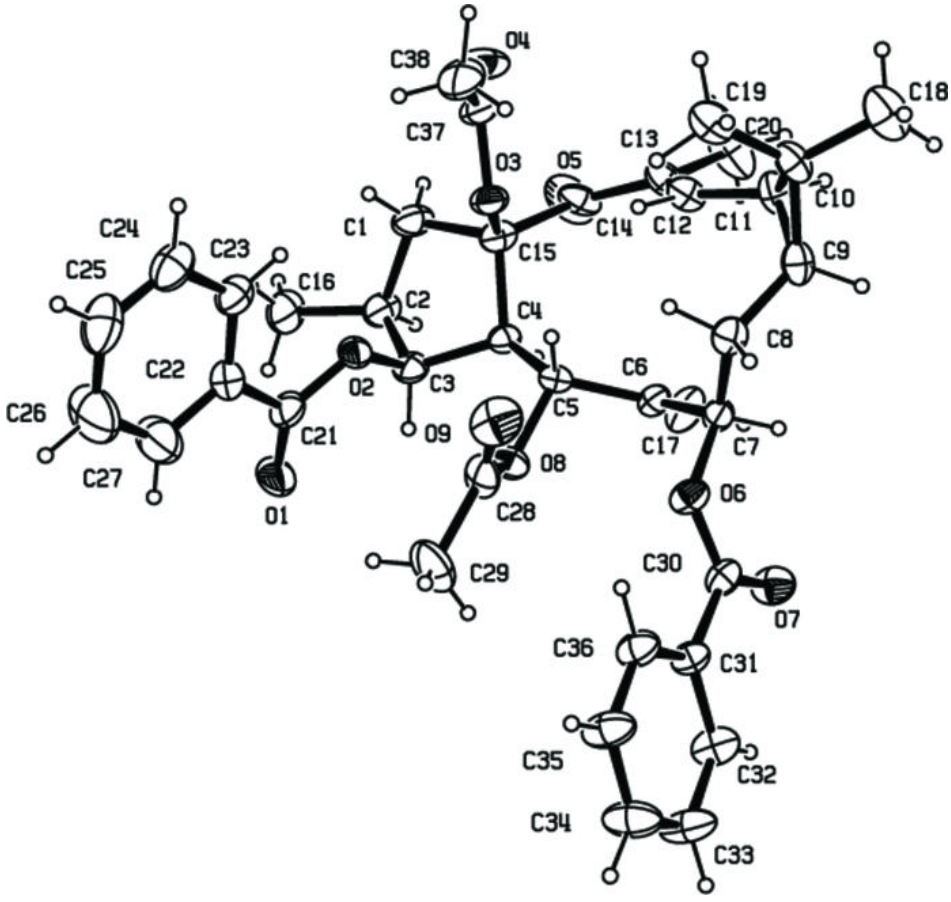
O4
C38
C37
C19
C18
C20
C13
O3
O5
C10
C1
C14
C12
C11
C24
C23
C15
C9
C25
C16
C2
C4
C8
C22
O2
C3
C6
C26
C5
C21
O9
C17
C7
C27
O8
O6
O1
C28
C29
C30
O7
C36
C31
C35
O2
C34
C33

Fig. 2