

6 α -Cinnamoyloxyeudesman-15-oic acidRenato Murillo,^a Alexander Briceño,^b Asiloé J. Mora^c and Gerzon E. Delgado^{c*}^aEscuela de Química and CIPRONA, Universidad de Costa Rica, San José, Costa Rica, ^bLaboratorio de Síntesis y Caracterización de Nuevos Materiales, IVIC, Caracas, Venezuela, and ^cLaboratorio de Cristalografía, Departamento de Química, Facultad de Ciencias, Universidad de Los Andes, Mérida 5101, Venezuela

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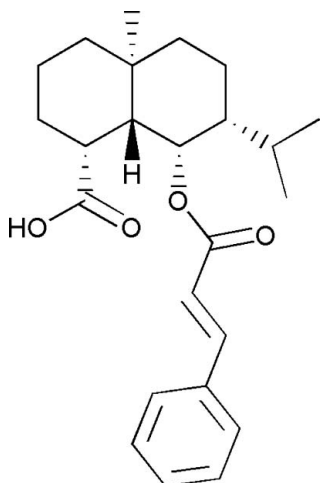
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.045; wR factor = 0.098; data-to-parameter ratio = 6.7.

The structure of the title compound [systematic name: (1*R*,4*aS*,7*R*,8*S*,*E*)-8-cinnamoyloxy-7-isopropyl-4*a*-methyl-decahydronaphthalene-1-carboxylic acid], $\text{C}_{24}\text{H}_{32}\text{O}_4$, isolated from *Verbesina turbacensis* collected in Costa Rica, shows a eudesman sesquiterpene skeleton with normal values of bond lengths and angles. In the crystal structure, the hydroxy group is involved in the formation of intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds, which link the molecules into zigzag chains extended along the [001] direction.

Related literature

The title compound was isolated in its ester and acid forms by Bohlmann & Lonitz (1978) and Amaro-Luis *et al.* (2002), respectively. For related literature concerning the sesquiterpene derivatives extracted from the Asteraceae family of plants, see: Castro *et al.* (2000); Amaro-Luis *et al.* (2002); Wagner *et al.* (2004); Stefani *et al.* (2006).



Experimental

Crystal data

$\text{C}_{24}\text{H}_{32}\text{O}_4$
 $M_r = 384.50$
 Orthorhombic, $P2_12_12_1$
 $a = 14.252$ (3) Å
 $b = 17.312$ (3) Å
 $c = 8.820$ (4) Å
 $V = 2176.1$ (11) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 293$ (2) K
 $0.40 \times 0.20 \times 0.10$ mm

Data collection

Rigaku AFC-7S diffractometer
 Absorption correction: none
 3559 measured reflections
 1697 independent reflections
 1060 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$
 3 standard reflections
 every 150 reflections
 intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.098$
 $S = 1.01$
 1697 reflections
 253 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.11$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.15$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1}\cdots\text{O4}^i$	0.82	1.96	2.760 (5)	167

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

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2242).

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supplementary materials

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6*O*-Cinnamoyloxyeudesman-15-oic acid

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Comment

Sesquiterpene derivatives are natural products responsible for the anti-inflammatory activity of a variety of medicinal plants, mainly from the Asteraceae family (Castro *et al.*, 2000; Amaro-Luis *et al.*, 2002; Wagner *et al.*, 2004; Stefani *et al.*, 2006). In particular, from the *Verbesina turbacensis* plant, collected in Costa Rica, were isolated the sesquiterpenes 15 ol derivate and the 15 oic derivate (I). The title compound (I), was reported in its ester's form, extracted from the *Verbesina eggersii* collected in Ecuador (Bohlmann & Lonitz, 1978) and later from *Verbesina turbacensis* collected in Venezuela (Amaro-Luis *et al.*, 2002). In the molecule, all bond lengths and angles are normal. The molecular structure of (I) (Fig. 1) shows that the A and B rings adopt the chair conformations [$\Delta C_2(2-3)_{\min} = 1.7$ (6), $\Delta C_2(3-4)_{\max} = 2.6$ (6), $\Delta C_s(2)_{\min} = 1.1$ (4), $\Delta C_s(1)_{\max} = 2.3$ (5)] for A and [$\Delta C_2(6-7)_{\min} = 3.9$ (6), $\Delta C_2(5-6)_{\max} = 5.2$ (6), $\Delta C_s(7)_{\min} = 0.5$ (5), $\Delta C_s(6)_{\max} = 4.6$ (5)] for B, respectively [Griffin, J. F., Duax, W. & Weeks, M. (1984). "Atlas of Steroid Structure". New York: Plenum Publishing corporation]. The crystal packing is stabilized by an O—H \cdots O hydrogen bond (Table 1). In the extended zigzag chains which run along the [001] direction, as depicted in Fig. 2, molecules are related by 2_1 screw axis, and are linked by hydrogen bonds; each molecule acting as a donor of a hydrogen atom through the carboxylic acid group, and as an acceptor of a hydrogen atom through the oxygen atom in the ester group. Hydrophobic groups are located in the outer region of each chain.

Experimental

The title compound (II) was isolated from aerial parts of *Verbesina turbacensis* (Asteraceae) in San José, Costa Rica in 2000. Crystals of (II) suitable for X-ray analysis were obtained by slow evaporation of an ethyl acetate solution at room temperature. ^1H NMR (400 MHz, DMSO- d_6): δ 1.39 (H1a, *m*), 1.00 (H1b, *m*), 1.88 (H2a, *m*), 1.24 (H2b, *m*), 1.48 (H3a, *m*), 1.14 (H3b, *m*), 2.32 (H4, *m*), 1.55 (H5, *dd*), 5.42 (H6, *dd*), 1.14 (H7, *m*), 1.50 (H8a, *m*), 1.60 (H8b, *m*), 1.55 (H9a, *m*), 1.12 (H9b, *m*), 1.42 (H11, *m*), 1.00 (H12, *d*), 0.81 (H13, *d*), 1.24 (H14, *s*), 6.33 (H17, *d*), 7.62 (H18, *d*), 7.50 (H20–24, *m*), 7.33 (H21–23, *m*), 7.33 (H22, *m*); ^{13}C NMR (100 MHz, DMSO- d_6): δ 44.1 (C1, *t*), 18.6 (C2, *t*), 29.8 (C3, *t*), 42.4 (C4, *d*), 50.4 (C5, *d*), 74.1 (C6, *d*), 51.0 (C7, *d*), 20.7 (C8, *d*), 44.4 (C9, *t*), 34.3 (C10, *s*), 28.2 (C11, *d*), 22.3 (C12, *q*), 202, (C13, *q*), 20.6 (C14, *q*), 166.7 (C16, *s*), 118.6 (C17, *d*), 144.1 (C18, *d*), 134.7 (C19, *s*), 128.1 (C20–24, *d*), 128.6 (C21–23, *d*), 129.7 (C22, *d*).

Refinement

All H atom attached to C atoms were positioned geometrically like idealized group and isotropic displacement parameters were set equal to 1.2 times $U_{\text{eq}}(\text{parent})$ or 1.5 $U_{\text{eq}}(\text{parent})$ (methyls). The hydroxy H atom was positioned geometrically [O—H 0.82 Å], and refined with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$. The absolute configuration was not established because of the absence of significant anomalous scatterers. 915 Friedel pairs were merged before the final refinement.

Figures

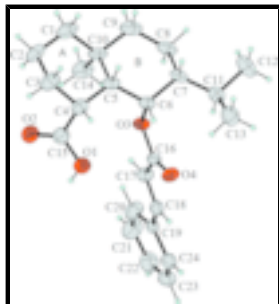


Fig. 1. **Figure 1.** View of (I) with the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown with an arbitrary radius.

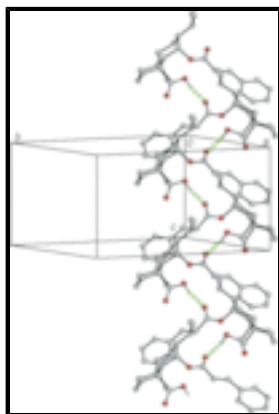


Fig. 2. **Figure 2.** A partial packing view of (I). Hydrogen bonds are marked with green, dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

(1*R*,4*aS*,7*R*,8*S*,*E*)-8-cinnamoxyl-7-isopropyl-4*a*-methyldecahydronaphthalene-1-carboxylic acid

Crystal data

$C_{24}H_{32}O_4$

$M_r = 384.50$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 14.252 (3) \text{ \AA}$

$b = 17.312 (3) \text{ \AA}$

$c = 8.820 (4) \text{ \AA}$

$V = 2176.1 (11) \text{ \AA}^3$

$Z = 4$

$F_{000} = 832$

$D_x = 1.174 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71069 \text{ \AA}$

Cell parameters from 20 reflections

$\theta = 1.8\text{--}24.8^\circ$

$\mu = 0.08 \text{ mm}^{-1}$

$T = 293 (2) \text{ K}$

Rectangular, colourless

$0.40 \times 0.20 \times 0.10 \text{ mm}$

Data collection

Rigaku AFC-7S
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293(2) \text{ K}$

ω - 2θ scans

Absorption correction: none

$R_{\text{int}} = 0.025$

$\theta_{\text{max}} = 25.0^\circ$

$\theta_{\text{min}} = 1.9^\circ$

$h = -3 \rightarrow 10$

$k = -3 \rightarrow 20$

$l = -3 \rightarrow 10$

3559 measured reflections
 1697 independent reflections
 1060 reflections with $I > 2\sigma(I)$

3 standard reflections
 every 150 reflections
 intensity decay: none

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.098$
 $S = 1.01$
 1697 reflections
 253 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
 $w = 1/[\sigma^2(F_o^2) + (0.0389P)^2 + 0.3391P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.11 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.15 \text{ e } \text{\AA}^{-3}$
 Extinction correction: none

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.1910 (3)	0.0954 (2)	0.4197 (4)	0.078 (1)
H1	0.2165	0.0779	0.4956	0.117*
O2	0.1115 (3)	0.1614 (2)	0.5900 (4)	0.0927 (14)
O3	0.0645 (2)	-0.00138 (16)	0.2568 (3)	0.0465 (9)
O4	0.2036 (2)	-0.02560 (16)	0.1437 (4)	0.0560 (10)
C1	-0.1312 (4)	0.1924 (3)	0.3740 (7)	0.0755 (19)
H1A	-0.1508	0.2205	0.2843	0.091*
H1B	-0.1865	0.1835	0.4356	0.091*
C2	-0.0636 (4)	0.2423 (3)	0.4624 (7)	0.0770 (18)
H2A	-0.0488	0.2173	0.5580	0.092*
H2B	-0.0929	0.2915	0.4847	0.092*
C3	0.0262 (4)	0.2557 (3)	0.3736 (6)	0.0727 (18)
H3A	0.0696	0.2852	0.4354	0.087*
H3B	0.0121	0.2859	0.2839	0.087*
C4	0.0734 (4)	0.1798 (2)	0.3256 (6)	0.0545 (15)

supplementary materials

H4	0.1220	0.1939	0.2521	0.065*
C5	0.0021 (4)	0.1291 (2)	0.2386 (6)	0.0488 (13)
H5	-0.0183	0.1638	0.1572	0.059*
C6	0.0416 (3)	0.0607 (2)	0.1502 (5)	0.0435 (13)
H6	0.0986	0.0767	0.0964	0.052*
C7	-0.0299 (3)	0.0289 (3)	0.0360 (5)	0.0507 (13)
H7	-0.0456	0.0716	-0.0323	0.061*
C8	-0.1198 (4)	0.0090 (3)	0.1220 (6)	0.0691 (16)
H8A	-0.1667	-0.0087	0.0502	0.083*
H8B	-0.1070	-0.0331	0.1915	0.083*
C9	-0.1592 (4)	0.0771 (4)	0.2109 (6)	0.0789 (18)
H9A	-0.2146	0.0599	0.2654	0.095*
H9B	-0.1790	0.1165	0.1396	0.095*
C10	-0.0909 (4)	0.1135 (3)	0.3245 (6)	0.0573 (15)
C11	0.0080 (4)	-0.0369 (3)	-0.0645 (6)	0.0602 (15)
H11	0.0342	-0.0768	0.0021	0.072*
C12	-0.0695 (4)	-0.0744 (3)	-0.1611 (6)	0.093 (2)
H12A	-0.1191	-0.0922	-0.0962	0.139*
H12B	-0.0439	-0.1173	-0.2164	0.139*
H12C	-0.0940	-0.0370	-0.2311	0.139*
C13	0.0865 (4)	-0.0087 (3)	-0.1692 (5)	0.0769 (17)
H13A	0.1097	-0.0512	-0.2282	0.115*
H13B	0.1367	0.0123	-0.1093	0.115*
H13C	0.0625	0.0305	-0.2356	0.115*
C14	-0.0817 (3)	0.0609 (3)	0.4648 (5)	0.0715 (17)
H14A	-0.0556	0.0121	0.4351	0.107*
H14B	-0.1426	0.0529	0.5087	0.107*
H14C	-0.0413	0.0850	0.5379	0.107*
C15	0.1245 (4)	0.1448 (3)	0.4604 (7)	0.0604 (15)
C16	0.1471 (4)	-0.0392 (3)	0.2424 (6)	0.0440 (13)
C17	0.1552 (3)	-0.0980 (2)	0.3611 (5)	0.0480 (13)
H17	0.1090	-0.1019	0.4351	0.058*
C18	0.2278 (4)	-0.1457 (2)	0.3642 (5)	0.0501 (14)
H18	0.2742	-0.1373	0.2918	0.060*
C19	0.2432 (4)	-0.2099 (2)	0.4681 (6)	0.0481 (13)
C20	0.1829 (4)	-0.2284 (3)	0.5827 (6)	0.0736 (17)
H20	0.1304	-0.1977	0.6002	0.088*
C21	0.1989 (5)	-0.2928 (3)	0.6737 (6)	0.087 (2)
H21	0.1574	-0.3048	0.7516	0.105*
C22	0.2754 (5)	-0.3382 (3)	0.6487 (7)	0.080 (2)
H22	0.2856	-0.3815	0.7087	0.096*
C23	0.3363 (4)	-0.3203 (3)	0.5370 (7)	0.0721 (17)
H23	0.3885	-0.3515	0.5209	0.086*
C24	0.3221 (4)	-0.2563 (3)	0.4465 (6)	0.0582 (15)
H24	0.3651	-0.2442	0.3709	0.070*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.079 (3)	0.081 (2)	0.073 (3)	0.030 (2)	-0.018 (2)	-0.011 (2)
O2	0.089 (3)	0.125 (3)	0.063 (2)	0.037 (3)	-0.007 (3)	-0.015 (3)
O3	0.039 (2)	0.0480 (17)	0.0520 (19)	0.0044 (18)	-0.0016 (19)	0.0176 (17)
O4	0.048 (3)	0.059 (2)	0.061 (2)	0.0099 (18)	0.007 (2)	0.0085 (19)
C1	0.068 (5)	0.078 (4)	0.081 (4)	0.031 (4)	0.019 (4)	0.022 (3)
C2	0.080 (5)	0.063 (3)	0.088 (4)	0.030 (3)	0.023 (4)	0.000 (4)
C3	0.081 (5)	0.049 (3)	0.089 (4)	0.015 (3)	0.013 (4)	0.007 (3)
C4	0.061 (4)	0.045 (3)	0.057 (3)	0.008 (3)	0.006 (3)	0.014 (3)
C5	0.043 (4)	0.047 (3)	0.056 (3)	0.008 (3)	-0.001 (3)	0.020 (3)
C6	0.035 (3)	0.046 (3)	0.049 (3)	-0.001 (2)	-0.006 (3)	0.017 (3)
C7	0.037 (4)	0.060 (3)	0.055 (3)	-0.008 (3)	-0.013 (3)	0.019 (3)
C8	0.040 (4)	0.088 (4)	0.079 (4)	-0.012 (3)	-0.014 (3)	0.012 (4)
C9	0.044 (5)	0.110 (5)	0.083 (4)	0.006 (4)	-0.001 (4)	0.023 (4)
C10	0.035 (4)	0.071 (3)	0.065 (3)	0.012 (3)	0.004 (4)	0.019 (3)
C11	0.063 (4)	0.059 (3)	0.058 (3)	-0.009 (3)	-0.010 (3)	0.005 (3)
C12	0.093 (5)	0.104 (4)	0.081 (4)	-0.030 (4)	-0.029 (4)	-0.005 (4)
C13	0.079 (5)	0.090 (4)	0.062 (3)	-0.013 (4)	0.001 (4)	0.003 (3)
C14	0.065 (4)	0.079 (3)	0.070 (3)	0.001 (3)	0.019 (4)	0.031 (3)
C15	0.056 (5)	0.054 (3)	0.071 (4)	-0.002 (3)	0.001 (4)	-0.004 (3)
C16	0.034 (4)	0.041 (3)	0.057 (3)	0.000 (3)	-0.008 (3)	-0.008 (3)
C17	0.048 (4)	0.041 (3)	0.055 (3)	0.003 (3)	-0.001 (3)	0.010 (3)
C18	0.059 (4)	0.042 (3)	0.049 (3)	0.001 (3)	-0.006 (3)	-0.006 (3)
C19	0.055 (4)	0.044 (3)	0.045 (3)	0.010 (3)	-0.016 (3)	-0.006 (3)
C20	0.092 (5)	0.066 (3)	0.063 (4)	0.030 (3)	0.013 (4)	0.012 (3)
C21	0.112 (6)	0.087 (4)	0.062 (4)	0.029 (4)	0.018 (4)	0.026 (4)
C22	0.112 (6)	0.060 (3)	0.068 (4)	0.016 (4)	-0.020 (4)	0.013 (4)
C23	0.077 (5)	0.059 (3)	0.080 (4)	0.021 (3)	-0.028 (4)	0.001 (4)
C24	0.059 (4)	0.058 (3)	0.058 (3)	0.004 (3)	-0.012 (3)	-0.001 (3)

Geometric parameters (\AA , $^\circ$)

O1—C15	1.326 (6)	C9—H9A	0.9700
O1—H1	0.8200	C9—H9B	0.9700
O2—C15	1.194 (6)	C10—C14	1.542 (6)
O3—C16	1.353 (5)	C11—C13	1.531 (6)
O3—C6	1.465 (4)	C11—C12	1.539 (6)
O4—C16	1.209 (5)	C11—H11	0.9800
C1—C2	1.510 (7)	C12—H12A	0.9600
C1—C10	1.545 (6)	C12—H12B	0.9600
C1—H1A	0.9700	C12—H12C	0.9600
C1—H1B	0.9700	C13—H13A	0.9600
C2—C3	1.519 (7)	C13—H13B	0.9600
C2—H2A	0.9700	C13—H13C	0.9600
C2—H2B	0.9700	C14—H14A	0.9600
C3—C4	1.535 (6)	C14—H14B	0.9600

supplementary materials

C3—H3A	0.9700	C14—H14C	0.9600
C3—H3B	0.9700	C16—C17	1.465 (6)
C4—C15	1.521 (7)	C17—C18	1.324 (6)
C4—C5	1.546 (6)	C17—H17	0.9300
C4—H4	0.9800	C18—C19	1.457 (6)
C5—C6	1.526 (6)	C18—H18	0.9300
C5—C10	1.550 (6)	C19—C20	1.366 (6)
C5—H5	0.9800	C19—C24	1.395 (6)
C6—C7	1.535 (6)	C20—C21	1.393 (7)
C6—H6	0.9800	C20—H20	0.9300
C7—C8	1.527 (6)	C21—C22	1.361 (7)
C7—C11	1.542 (6)	C21—H21	0.9300
C7—H7	0.9800	C22—C23	1.349 (7)
C8—C9	1.523 (6)	C22—H22	0.9300
C8—H8A	0.9700	C23—C24	1.381 (6)
C8—H8B	0.9700	C23—H23	0.9300
C9—C10	1.533 (7)	C24—H24	0.9300
C15—O1—H1	109.5	C14—C10—C1	109.0 (4)
C16—O3—C6	119.2 (4)	C9—C10—C5	107.2 (4)
C2—C1—C10	114.5 (5)	C14—C10—C5	115.0 (4)
C2—C1—H1A	108.6	C1—C10—C5	107.5 (4)
C10—C1—H1A	108.6	C13—C11—C12	109.0 (4)
C2—C1—H1B	108.6	C13—C11—C7	111.5 (4)
C10—C1—H1B	108.6	C12—C11—C7	112.2 (4)
H1A—C1—H1B	107.6	C13—C11—H11	108.0
C1—C2—C3	111.0 (5)	C12—C11—H11	108.0
C1—C2—H2A	109.4	C7—C11—H11	108.0
C3—C2—H2A	109.4	C11—C12—H12A	109.5
C1—C2—H2B	109.4	C11—C12—H12B	109.5
C3—C2—H2B	109.4	H12A—C12—H12B	109.5
H2A—C2—H2B	108.0	C11—C12—H12C	109.5
C2—C3—C4	112.3 (4)	H12A—C12—H12C	109.5
C2—C3—H3A	109.1	H12B—C12—H12C	109.5
C4—C3—H3A	109.1	C11—C13—H13A	109.5
C2—C3—H3B	109.1	C11—C13—H13B	109.5
C4—C3—H3B	109.1	H13A—C13—H13B	109.5
H3A—C3—H3B	107.9	C11—C13—H13C	109.5
C15—C4—C3	109.6 (5)	H13A—C13—H13C	109.5
C15—C4—C5	118.5 (4)	H13B—C13—H13C	109.5
C3—C4—C5	109.6 (4)	C10—C14—H14A	109.5
C15—C4—H4	106.1	C10—C14—H14B	109.5
C3—C4—H4	106.1	H14A—C14—H14B	109.5
C5—C4—H4	106.1	C10—C14—H14C	109.5
C6—C5—C4	116.8 (4)	H14A—C14—H14C	109.5
C6—C5—C10	115.4 (4)	H14B—C14—H14C	109.5
C4—C5—C10	114.7 (4)	O2—C15—O1	121.7 (5)
C6—C5—H5	102.2	O2—C15—C4	125.4 (5)
C4—C5—H5	102.2	O1—C15—C4	112.8 (5)
C10—C5—H5	102.2	O4—C16—O3	123.5 (4)

O3—C6—C5	108.9 (3)	O4—C16—C17	126.7 (5)
O3—C6—C7	107.8 (3)	O3—C16—C17	109.8 (5)
C5—C6—C7	111.6 (4)	C18—C17—C16	120.6 (5)
O3—C6—H6	109.5	C18—C17—H17	119.7
C5—C6—H6	109.5	C16—C17—H17	119.7
C7—C6—H6	109.5	C17—C18—C19	127.3 (5)
C8—C7—C6	108.2 (4)	C17—C18—H18	116.3
C8—C7—C11	114.4 (4)	C19—C18—H18	116.3
C6—C7—C11	114.2 (4)	C20—C19—C24	118.2 (5)
C8—C7—H7	106.5	C20—C19—C18	123.3 (5)
C6—C7—H7	106.5	C24—C19—C18	118.4 (5)
C11—C7—H7	106.5	C19—C20—C21	120.7 (5)
C9—C8—C7	113.0 (4)	C19—C20—H20	119.6
C9—C8—H8A	109.0	C21—C20—H20	119.6
C7—C8—H8A	109.0	C22—C21—C20	120.0 (6)
C9—C8—H8B	109.0	C22—C21—H21	120.0
C7—C8—H8B	109.0	C20—C21—H21	120.0
H8A—C8—H8B	107.8	C23—C22—C21	120.1 (5)
C8—C9—C10	114.8 (4)	C23—C22—H22	119.9
C8—C9—H9A	108.6	C21—C22—H22	119.9
C10—C9—H9A	108.6	C22—C23—C24	120.7 (6)
C8—C9—H9B	108.6	C22—C23—H23	119.6
C10—C9—H9B	108.6	C24—C23—H23	119.6
H9A—C9—H9B	107.5	C23—C24—C19	120.2 (5)
C9—C10—C14	109.6 (4)	C23—C24—H24	119.9
C9—C10—C1	108.2 (5)	C19—C24—H24	119.9

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots O4 ⁱ	0.82	1.96	2.760 (5)	167

Symmetry codes: (i) $-x+1/2, -y, z+1/2$.

Fig. 1

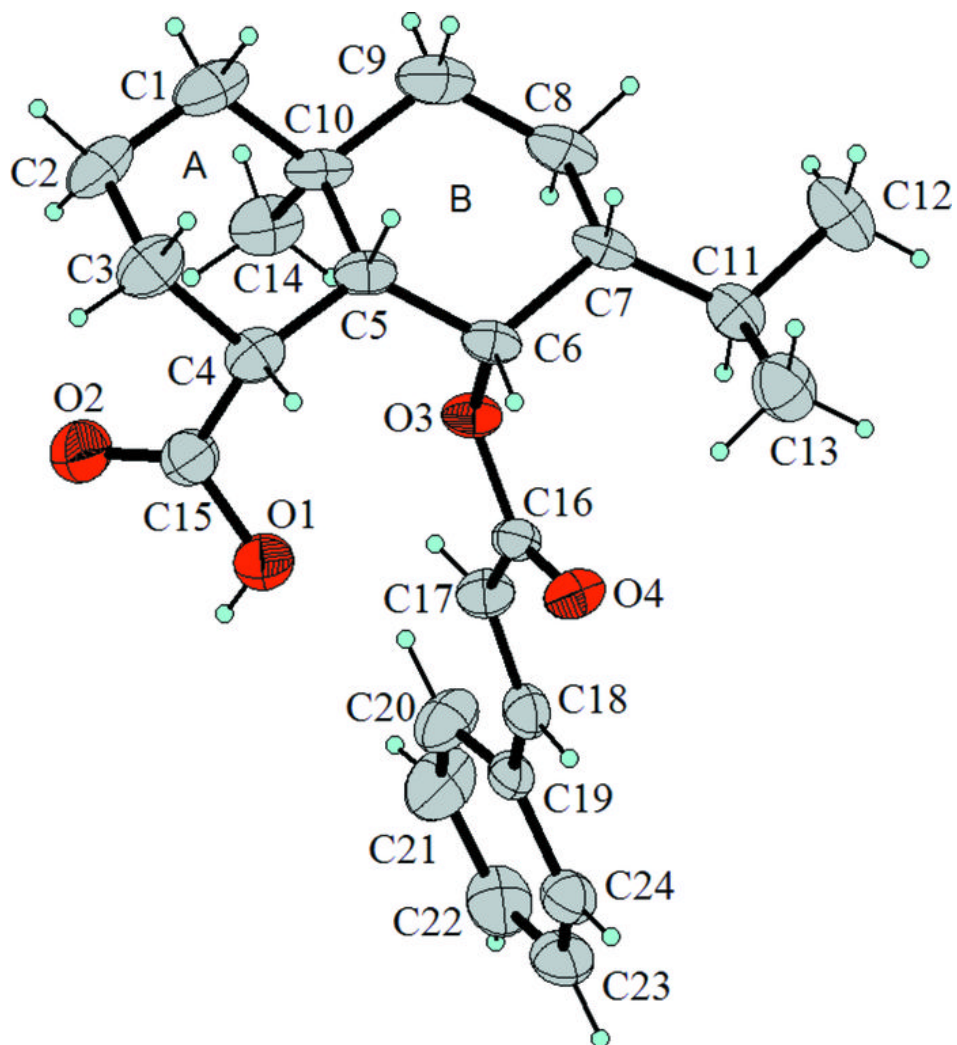


Fig. 2

