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ent-Kaur-16-en-19-al

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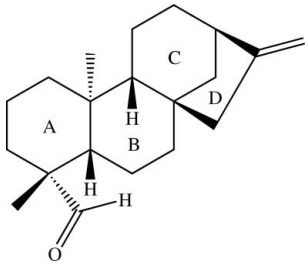
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.097; data-to-parameter ratio = 14.1.

The title *ent*-kaurane diterpene compound, $C_{20}H_{30}O$, was isolated from the roots of *Bruguiera cylindrica* (Rhizophoraceae), a mangrove plant. The molecule contains a fused four-ring system, with the three cyclohexane rings in standard chair conformations and the cyclopentane ring adopting an envelope conformation. The aldehyde is bisectionally attached to the cyclohexane ring. The methylene group is coplanar with the attached cyclopentane ring. In the crystal structure, molecules are packed by van der Waals interactions.

Related literature

For the values of bond lengths, see Allen *et al.* (1987). For literature on ring conformations, see Cremer & Pople (1975). For further details of *ent*-kaurane diterpenes and their bioactive properties, see, for example: Karle (1972); Müller *et al.* (2003); Salae *et al.* (2007).



Experimental

Crystal data

$C_{20}H_{30}O$
M_r = 286.44
Orthorhombic, $P2_12_12_1$
a = 6.3126 (2) Å
b = 11.2823 (4) Å
c = 22.8044 (7) Å
V = 1624.14 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 100.0 (1) K
0.56 × 0.40 × 0.13 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.952, T_{max} = 0.991
20475 measured reflections
2709 independent reflections
2571 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.097
S = 1.07
2709 reflections
192 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2036).

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supplementary materials

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ent-Kaur-16-en-19-al

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Comment

The title *ent*-kaurane compound, known as *ent*-kaur-16-ene-19-al, was isolated from the roots of *Bruguiera cylindrica* (Rhizophoraceae), a mangrove plant which was found in South East Asia. In our continuing research on bioactive compounds from mangrove sources, we have studied the chemical constituents from the roots of *Bruguiera cylindrica* (Rhizophoraceae) to search for the bioactive components. We have previously reported the crystal structure of the *ent*-kaur-16-ene-13,19-diol which was isolated from this plant (Salae *et al.*, 2007). We herein report the crystal structure of the title compound which has an inhibitory activity on vascular smooth muscle contraction (Müller *et al.*, 2003).

The molecule of the title compound contains a fused four-ring system *A/B/C/D* (Scheme 1). The *A/B* ring junction is *trans*-fused, *B/C* and *C/D* are *cis*-fused (Fig. 1). The three cyclohexane rings has the standard chair conformations; the cyclopentane ring adopts an envelope conformation with atom C14 displaced from the C8/C15/C16/C13 plane by −0.2891 (14) Å, and with puckering parameters (Cremer & Pople, 1975) Q = 0.459 (1) Å and φ = 30.35 (18)°. The methylene group is planarly attached to cyclopentane ring at atom C16. The bond angles around C16 are indicative of sp^2 hybridization for these atoms, with the geometric parameters being given in the supplementary materials. The orientation of the aldehyde group can be indicated by the torsion angles C3–C4–C19–O1 = −16.3 (2)° and C5–C4–C19–O1 = −140.60((15)°. All bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and comparable to the closely related structure *ent*-Kaur-16-ene-13,19-diol (Salae *et al.*, 2007). The title structure is isomorphous to *ent*-Kaur-15-ene-19-al (Karle, 1972) and these two structures crystallized out in the same space group and have almost identical unit-cell dimensions. The differences in these two structures are that in the structure of *ent*-Kaur-15-ene-19-al, the functional group attached to C16 is a methyl group and C15—C16 is a C═C bond. The origins of the structures are different; *ent*-Kaur-15-ene-19-al was isolated from the tubers of *Espeelita weddeli*, a Composita which grows at 10,0000 feet in the Venezuelan Andes.

In the crystal packing of the title compound, the molecules are packed by Van de Waals interactions (Fig. 2).

Experimental

The air-dried roots of *Bruguiera cylindrica* (6.0 kg) were chopped and extracted with CH_2Cl_2 (2 *x* 22 l) for one week at room temperature. Removal of the solvent from CH_2Cl_2 extract under reduced pressure gave a yellow viscous residue (38.5 g) which was subjected to quick column chromatography over siliga gel using solvents of increasing polarity from n-hexane through EtOAc to afford 14 fractions (F1—F14). Fraction F6 was further separated by quick column chromatography using CH_2Cl_2-acetone (9:1) to give title compound (11.8 mg). Colorless plate-shaped single crystals of the title compound were recrystallized from n-hexane after several days [Mp. 387–388 K].

Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with the C—H distances in the range 0.93–0.98 Å. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups. A total of 2009 Friedel pairs were merged before final refinement as there is no large anomalous dispersion for the determination of the absolute configuration.

Figures

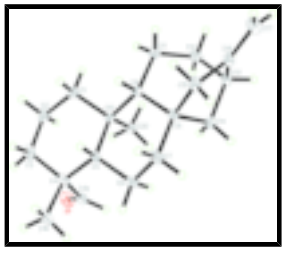

Fig. 1. The asymmetric unit of the title compound, showing 40% probability displacement ellipsoids and the atomic numbering scheme.

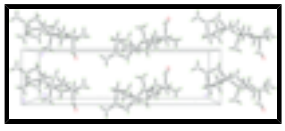

Fig. 2. The crystal packing of the title compound view along the *b* axis.

ent-Kaur-16-en-19-al

Crystal data

$C_{20}H_{30}O$	$D_x = 1.171$ Mg m^{-3}
$M_r = 286.44$	Melting point: 387-388 K
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 2709 reflections
$a = 6.3126$ (2) Å	$\theta = 1.8$–$30.0°$
$b = 11.2823$ (4) Å	$\mu = 0.07$ mm^{-1}
$c = 22.8044$ (7) Å	$T = 100.0$ (1) K
$V = 1624.14$ (9) Å^3	Plate, colorless
$Z = 4$	0.56 × 0.40 × 0.13 mm
$F_{000} = 632$	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	2709 independent reflections
Radiation source: fine-focus sealed tube	2571 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.029$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 30.0°$
$T = 100.0(1)$ K	$\theta_{min} = 1.8°$
ω scans	$h = -8 \rightarrow 8$

Absorption correction: multi-scan (SADABS; Bruker, 2005)

T_{min} = 0.952, T_{max} = 0.991

20475 measured reflections

k = −14→15

l = −27→32

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.035

$wR(F^2)$ = 0.097

S = 1.07

2709 reflections

192 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

$w = 1/[\sigma^2(F_o^2) + (0.0597P)^2 + 0.215P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max}$ = 0.31 e Å^{-3}

$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Extinction correction: none

Special details

Experimental. The low-temparture data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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 $F^2 > 2$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	0.34848 (17)	0.85293 (11)	0.74695 (5)	0.0330 (3)
C1	0.8278 (2)	0.73642 (11)	0.86634 (6)	0.0228 (3)
H1A	0.9792	0.7263	0.8610	0.027*
H1B	0.7863	0.6914	0.9007	0.027*
C2	0.7129 (3)	0.68629 (12)	0.81270 (7)	0.0284 (3)
H2A	0.7555	0.6045	0.8068	0.034*
H2B	0.5614	0.6874	0.8197	0.034*
C3	0.7620 (2)	0.75744 (14)	0.75763 (6)	0.0274 (3)
H3A	0.6761	0.7275	0.7256	0.033*
H3B	0.9095	0.7455	0.7472	0.033*
C4	0.7209 (2)	0.89086 (13)	0.76445 (6)	0.0204 (3)

C5	0.8351 (2)	0.93785 (11)	0.82017 (5)	0.0169 (2)
H5A	0.9856	0.9216	0.8133	0.020*
C6	0.8231 (2)	1.07270 (12)	0.82971 (6)	0.0215 (3)
H6A	0.8473	1.1135	0.7929	0.026*
H6B	0.6834	1.0942	0.8439	0.026*
C7	0.9906 (2)	1.10943 (12)	0.87436 (6)	0.0226 (3)
H7A	0.9862	1.1948	0.8793	0.027*
H7B	1.1296	1.0886	0.8595	0.027*
C8	0.9579 (2)	1.05008 (11)	0.93396 (5)	0.0163 (2)
C9	0.93310 (19)	0.91333 (11)	0.92681 (5)	0.0150 (2)
H9A	1.0735	0.8860	0.9145	0.018*
C10	0.78062 (19)	0.86948 (11)	0.87740 (5)	0.0153 (2)
C11	0.8994 (2)	0.85560 (11)	0.98797 (6)	0.0190 (2)
H11A	0.8348	0.7785	0.9821	0.023*
H11B	1.0374	0.8425	1.0055	0.023*
C12	0.7633 (2)	0.92480 (12)	1.03200 (6)	0.0218 (3)
H12A	0.7859	0.8932	1.0711	0.026*
H12B	0.6148	0.9147	1.0223	0.026*
C13	0.8187 (2)	1.05776 (12)	1.03149 (6)	0.0198 (3)
H13A	0.7411	1.1021	1.0616	0.024*
C14	0.7751 (2)	1.10491 (11)	0.96959 (6)	0.0199 (3)
H14A	0.7801	1.1908	0.9685	0.024*
H14B	0.6385	1.0784	0.9552	0.024*
C15	1.1454 (2)	1.07505 (12)	0.97590 (6)	0.0218 (3)
H15A	1.2538	1.0148	0.9715	0.026*
H15B	1.2076	1.1518	0.9674	0.026*
C16	1.0568 (2)	1.07321 (12)	1.03703 (6)	0.0204 (3)
C17	1.1674 (3)	1.08212 (14)	1.08712 (6)	0.0282 (3)
H17A	1.3140	1.0904	1.0859	0.034*
H17B	1.0975	1.0800	1.1230	0.034*
C18	0.8071 (3)	0.95405 (17)	0.70911 (6)	0.0318 (4)
H18A	0.7532	0.9155	0.6747	0.048*
H18B	0.9590	0.9505	0.7090	0.048*
H18C	0.7624	1.0354	0.7093	0.048*
C19	0.4858 (2)	0.91868 (14)	0.76388 (6)	0.0230 (3)
H19A	0.4442	0.9926	0.7777	0.028*
C20	0.5454 (2)	0.88135 (11)	0.89396 (6)	0.0178 (2)
H20A	0.4606	0.8382	0.8663	0.027*
H20B	0.5056	0.9635	0.8933	0.027*
H20C	0.5233	0.8498	0.9326	0.027*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0191 (5)	0.0504 (7)	0.0296 (6)	0.0000 (5)	−0.0040 (4)	−0.0031 (5)
C1	0.0265 (7)	0.0165 (5)	0.0254 (6)	0.0048 (5)	−0.0092 (5)	−0.0052 (5)
C2	0.0320 (8)	0.0205 (6)	0.0325 (7)	0.0043 (6)	−0.0107 (6)	−0.0108 (5)
C3	0.0225 (6)	0.0354 (8)	0.0243 (7)	0.0058 (6)	−0.0040 (6)	−0.0143 (6)

C4	0.0164 (5)	0.0303 (7)	0.0144 (5)	0.0014 (5)	−0.0002 (4)	−0.0027 (5)
C5	0.0153 (5)	0.0217 (5)	0.0136 (5)	0.0006 (5)	0.0016 (4)	−0.0018 (4)
C6	0.0270 (6)	0.0209 (6)	0.0166 (6)	−0.0025 (5)	0.0017 (5)	0.0045 (5)
C7	0.0300 (7)	0.0211 (6)	0.0168 (6)	−0.0074 (5)	0.0040 (5)	0.0018 (5)
C8	0.0192 (5)	0.0154 (5)	0.0141 (5)	−0.0026 (5)	0.0027 (4)	−0.0004 (4)
C9	0.0152 (5)	0.0151 (5)	0.0149 (5)	0.0006 (4)	−0.0003 (4)	−0.0006 (4)
C10	0.0150 (5)	0.0149 (5)	0.0160 (5)	0.0011 (4)	−0.0006 (4)	−0.0005 (4)
C11	0.0221 (6)	0.0162 (5)	0.0187 (5)	−0.0013 (5)	−0.0050 (5)	0.0031 (5)
C12	0.0226 (6)	0.0264 (6)	0.0163 (5)	−0.0060 (5)	0.0011 (5)	0.0045 (5)
C13	0.0219 (6)	0.0228 (6)	0.0148 (5)	−0.0006 (5)	0.0042 (5)	−0.0029 (5)
C14	0.0258 (6)	0.0165 (5)	0.0173 (5)	0.0038 (5)	0.0032 (5)	−0.0020 (4)
C15	0.0229 (6)	0.0221 (6)	0.0204 (6)	−0.0075 (5)	0.0025 (5)	−0.0045 (5)
C16	0.0238 (6)	0.0181 (6)	0.0192 (6)	−0.0043 (5)	0.0035 (5)	−0.0026 (5)
C17	0.0294 (7)	0.0338 (7)	0.0215 (6)	−0.0074 (6)	0.0001 (6)	−0.0002 (6)
C18	0.0256 (7)	0.0556 (10)	0.0144 (6)	−0.0045 (7)	0.0025 (5)	−0.0005 (6)
C19	0.0196 (6)	0.0338 (7)	0.0156 (6)	0.0051 (6)	−0.0003 (5)	0.0016 (5)
C20	0.0154 (5)	0.0207 (6)	0.0173 (6)	−0.0014 (5)	0.0008 (4)	0.0020 (5)

Geometric parameters (Å, °)

O1—C19	1.2043 (19)	C9—C10	1.5625 (17)
C1—C2	1.5304 (19)	C9—H9A	0.9800
C1—C10	1.5511 (17)	C10—C20	1.5378 (17)
C1—H1A	0.9700	C11—C12	1.5350 (19)
C1—H1B	0.9700	C11—H11A	0.9700
C2—C3	1.522 (2)	C11—H11B	0.9700
C2—H2A	0.9700	C12—C13	1.5403 (18)
C2—H2B	0.9700	C12—H12A	0.9700
C3—C4	1.535 (2)	C12—H12B	0.9700
C3—H3A	0.9700	C13—C16	1.519 (2)
C3—H3B	0.9700	C13—C14	1.5333 (18)
C4—C19	1.5169 (19)	C13—H13A	0.9800
C4—C18	1.548 (2)	C14—H14A	0.9700
C4—C5	1.5543 (17)	C14—H14B	0.9700
C5—C6	1.5388 (18)	C15—C16	1.5020 (18)
C5—C10	1.5545 (17)	C15—H15A	0.9700
C5—H5A	0.9800	C15—H15B	0.9700
C6—C7	1.525 (2)	C16—C17	1.343 (2)
C6—H6A	0.9700	C17—H17A	0.9300
C6—H6B	0.9700	C17—H17B	0.9300
C7—C8	1.5291 (17)	C18—H18A	0.9600
C7—H7A	0.9700	C18—H18B	0.9600
C7—H7B	0.9700	C18—H18C	0.9600
C8—C14	1.5409 (18)	C19—H19A	0.9300
C8—C15	1.5475 (19)	C20—H20A	0.9600
C8—C9	1.5593 (16)	C20—H20B	0.9600
C9—C11	1.5538 (17)	C20—H20C	0.9600
C2—C1—C10	113.36 (11)	C1—C10—C5	107.53 (10)
C2—C1—H1A	108.9	C20—C10—C9	112.95 (10)

C10—C1—H1A	108.9	C1—C10—C9	107.78 (10)
C2—C1—H1B	108.9	C5—C10—C9	108.19 (10)
C10—C1—H1B	108.9	C12—C11—C9	116.78 (10)
H1A—C1—H1B	107.7	C12—C11—H11A	108.1
C3—C2—C1	111.59 (12)	C9—C11—H11A	108.1
C3—C2—H2A	109.3	C12—C11—H11B	108.1
C1—C2—H2A	109.3	C9—C11—H11B	108.1
C3—C2—H2B	109.3	H11A—C11—H11B	107.3
C1—C2—H2B	109.3	C11—C12—C13	111.30 (11)
H2A—C2—H2B	108.0	C11—C12—H12A	109.4
C2—C3—C4	113.52 (11)	C13—C12—H12A	109.4
C2—C3—H3A	108.9	C11—C12—H12B	109.4
C4—C3—H3A	108.9	C13—C12—H12B	109.4
C2—C3—H3B	108.9	H12A—C12—H12B	108.0
C4—C3—H3B	108.9	C16—C13—C14	102.38 (11)
H3A—C3—H3B	107.7	C16—C13—C12	109.62 (12)
C19—C4—C3	111.56 (12)	C14—C13—C12	107.71 (11)
C19—C4—C18	103.98 (12)	C16—C13—H13A	112.2
C3—C4—C18	108.03 (12)	C14—C13—H13A	112.2
C19—C4—C5	112.98 (11)	C12—C13—H13A	112.2
C3—C4—C5	109.80 (11)	C13—C14—C8	102.23 (10)
C18—C4—C5	110.25 (11)	C13—C14—H14A	111.3
C6—C5—C4	115.46 (11)	C8—C14—H14A	111.3
C6—C5—C10	111.16 (10)	C13—C14—H14B	111.3
C4—C5—C10	114.48 (11)	C8—C14—H14B	111.3
C6—C5—H5A	104.8	H14A—C14—H14B	109.2
C4—C5—H5A	104.8	C16—C15—C8	106.65 (11)
C10—C5—H5A	104.8	C16—C15—H15A	110.4
C7—C6—C5	109.20 (11)	C8—C15—H15A	110.4
C7—C6—H6A	109.8	C16—C15—H15B	110.4
C5—C6—H6A	109.8	C8—C15—H15B	110.4
C7—C6—H6B	109.8	H15A—C15—H15B	108.6
C5—C6—H6B	109.8	C17—C16—C15	126.52 (13)
H6A—C6—H6B	108.3	C17—C16—C13	126.46 (13)
C6—C7—C8	112.39 (11)	C15—C16—C13	107.02 (12)
C6—C7—H7A	109.1	C16—C17—H17A	120.0
C8—C7—H7A	109.1	C16—C17—H17B	120.0
C6—C7—H7B	109.1	H17A—C17—H17B	120.0
C8—C7—H7B	109.1	C4—C18—H18A	109.5
H7A—C7—H7B	107.9	C4—C18—H18B	109.5
C7—C8—C14	113.20 (11)	H18A—C18—H18B	109.5
C7—C8—C15	111.50 (11)	C4—C18—H18C	109.5
C14—C8—C15	100.00 (10)	H18A—C18—H18C	109.5
C7—C8—C9	110.73 (10)	H18B—C18—H18C	109.5
C14—C8—C9	112.16 (10)	O1—C19—C4	125.40 (14)
C15—C8—C9	108.75 (10)	O1—C19—H19A	117.3
C11—C9—C8	109.56 (10)	C4—C19—H19A	117.3
C11—C9—C10	115.49 (10)	C10—C20—H20A	109.5
C8—C9—C10	116.78 (10)	C10—C20—H20B	109.5

C11—C9—H9A	104.5	H20A—C20—H20B	109.5
C8—C9—H9A	104.5	C10—C20—H20C	109.5
C10—C9—H9A	104.5	H20A—C20—H20C	109.5
C20—C10—C1	108.04 (11)	H20B—C20—H20C	109.5
C20—C10—C5	112.13 (10)		
C10—C1—C2—C3	55.54 (17)	C6—C5—C10—C9	−55.86 (13)
C1—C2—C3—C4	−53.27 (17)	C4—C5—C10—C9	171.08 (10)
C2—C3—C4—C19	−74.39 (16)	C11—C9—C10—C20	54.39 (14)
C2—C3—C4—C18	171.92 (12)	C8—C9—C10—C20	−76.59 (14)
C2—C3—C4—C5	51.65 (16)	C11—C9—C10—C1	−64.88 (13)
C19—C4—C5—C6	−59.68 (16)	C8—C9—C10—C1	164.13 (11)
C3—C4—C5—C6	175.09 (11)	C11—C9—C10—C5	179.12 (10)
C18—C4—C5—C6	56.18 (15)	C8—C9—C10—C5	48.13 (13)
C19—C4—C5—C10	71.32 (15)	C8—C9—C11—C12	37.63 (15)
C3—C4—C5—C10	−53.91 (14)	C10—C9—C11—C12	−96.71 (13)
C18—C4—C5—C10	−172.82 (12)	C9—C11—C12—C13	−42.84 (16)
C4—C5—C6—C7	−163.78 (11)	C11—C12—C13—C16	−50.07 (15)
C10—C5—C6—C7	63.65 (14)	C11—C12—C13—C14	60.58 (14)
C5—C6—C7—C8	−60.81 (15)	C16—C13—C14—C8	43.12 (12)
C6—C7—C8—C14	−75.83 (14)	C12—C13—C14—C8	−72.41 (13)
C6—C7—C8—C15	172.33 (11)	C7—C8—C14—C13	−163.78 (11)
C6—C7—C8—C9	51.10 (15)	C15—C8—C14—C13	−45.06 (12)
C7—C8—C9—C11	−179.80 (11)	C9—C8—C14—C13	70.04 (13)
C14—C8—C9—C11	−52.29 (14)	C7—C8—C15—C16	150.54 (11)
C15—C8—C9—C11	57.36 (13)	C14—C8—C15—C16	30.58 (13)
C7—C8—C9—C10	−46.11 (15)	C9—C8—C15—C16	−87.08 (12)
C14—C8—C9—C10	81.39 (13)	C8—C15—C16—C17	174.74 (14)
C15—C8—C9—C10	−168.96 (10)	C8—C15—C16—C13	−4.54 (14)
C2—C1—C10—C20	66.22 (15)	C14—C13—C16—C17	157.01 (14)
C2—C1—C10—C5	−55.00 (15)	C12—C13—C16—C17	−88.85 (17)
C2—C1—C10—C9	−171.42 (12)	C14—C13—C16—C15	−23.71 (14)
C6—C5—C10—C20	69.36 (14)	C12—C13—C16—C15	90.43 (13)
C4—C5—C10—C20	−63.70 (14)	C3—C4—C19—O1	−16.3 (2)
C6—C5—C10—C1	−172.01 (11)	C18—C4—C19—O1	99.86 (17)
C4—C5—C10—C1	54.93 (14)	C5—C4—C19—O1	−140.60 (15)

Fig. 1

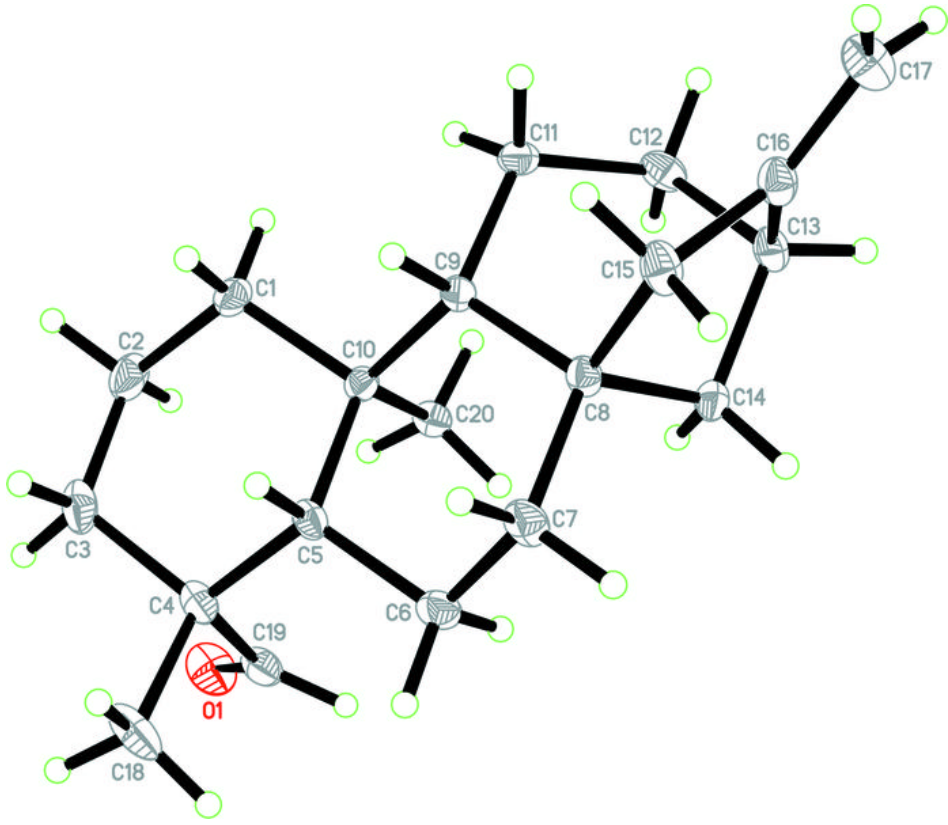
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Fig. 2