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Guidongnin A, a natural diterpenoid

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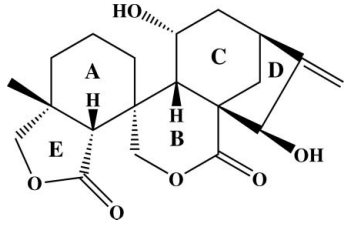
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.011 Å; R factor = 0.078; wR factor = 0.237; data-to-parameter ratio = 7.5.

The title compound, $C_{20}H_{26}O_6$, isolated from *Rabdosia var lophanthoides Hara*, is built up from five fused rings. The cyclohexane 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 *D* and *E* adopt envelope conformations. The isobenzofuran ring system couples orthogonally to the methanocyclohepta[*c*]pyran unit through a spiro C atom. The asymmetric unit consists of two unique molecules linked by hydrogen bonds to form a dimer. The dimers are further interconnected through O—H···O hydrogen bonds.

Related literature

For information on ring puckering analysis, see: Cremer & Pople (1975). For previous isolation of the title compound, see: Sun *et al.* (1988).



Experimental

Crystal data

$C_{20}H_{26}O_6$
M_r = 362.41
Orthorhombic, $P2_12_12_1$
a = 12.2614 (15) Å
b = 15.6668 (18) Å
c = 18.697 (2) Å
V = 3591.7 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.41 × 0.30 × 0.28 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.961, T_{max} = 0.973
17440 measured reflections
3556 independent reflections
1970 reflections with $I > 2\sigma(I)$
R_{int} = 0.084

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.078
$wR(F^2)$ = 0.237
S = 1.10
3556 reflections
472 parameters
1896 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O3*A*	0.82	2.46	3.159 (8)	144
O4*A*—H4*A*···O3	0.82	1.94	2.750 (8)	168
O5—H5···O3*A*^{i}	0.82	1.97	2.787 (8)	175
O5*A*—H5*B*···O6*A*^{ii}	0.82	2.11	2.903 (9)	164

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, -z$.

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: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2433).

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supplementary materials

Acta Cryst. (2007). E**63**, o4890 [**doi:10.1107/S1600536807060965**]

Guidongnin A, a natural diterpenoid

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Comment

The diterpenoid Guidongnin A, $C_{20}H_{26}O_6$, has been previously isolated from Rabdosia rubescens Hara (Sun *et al.*, 1988), its structure was established from the spectral and chemical evidence. Recently we isolated the compound from Rabdosia var lophanthoides Hara for the first time, and its structure is confirmed by an X-ray diffraction study.

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 (A,B,*C*,A',B'and C') and two five membered rings (D,*E*,D' and E'). The conformations of the different rings extracted from the puckering parameters (Cremer & Pople, 1975) are given in Table 2. Ring A and A' adopt a chair conformation, ring B and B' exist in a screw-boat conformation and rings C and C' adopt a boat conformation. Rings D, D', E and E' adopt an envelope conformation. The isobenzofuran ring system couples orthogonally to the methanocyclohepta[*c*] pyran moiety through a spiro C atom.

This two molecules are linked by O4—H4···O3A and O4A—H4A···O3 hydrogen bonds to form a dimer. The dimers are further interconnected through O—H···O hydrogen bonds (Fig.3).

Experimental

2 kg of dried powder from the whole plant, Rabdosia var lophanthoides Hara, was soaked three times with 95% EtOH at room temperature. The ethanolic extracts were evaporated under reduced pressure and the residue was successively fractionated with petroleum ether, EtOAc and n-BuOH. The residue of the petroleum ether fraction was subjected to column chromatography over silica gel. The column was eluted with a petroleum ether-EtOAc mixture and the title compound isolated. Crystals suitable for X-ray structure analysis were obtained by slow evaporation from a solution of methanol at room temperature.

Refinement

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).

In the absence of significant anomalous scattering, the absolute configuration could not be reliably determined from the X-ray analyses and the Friedel pairs were merged; stereochemistry was assigned following the work of Sun *et al.* (1988).

Figures

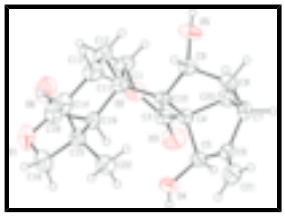

Fig. 1. Molecular view of molecule 1 with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres with arbitrary radii.

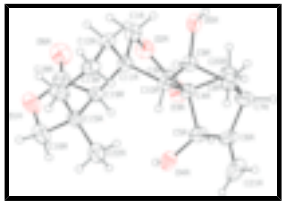

Fig. 2. Molecular view of molecule 2 with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres with arbitrary radii.

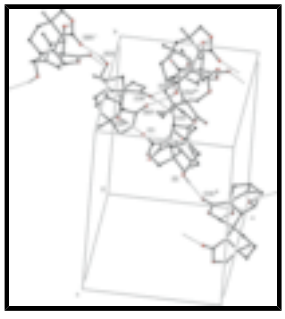

Fig. 3. Partial packing view of the title compound showing O—H···O hydrogen bonding interactions. H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry operations are assigned as follows: for atoms labelled with primes ('), (−1/2 + *x*, 3/2 − *y*, −*z*), asterisks (*) (1 − *x*, −1/2 + *y*, 1/2 − *z*), hashes (#) (−*x* + 1, 1/2 + *y*, 1/2 − *z*) and dollar signs ($) (1/2 + *x*, 3/2 − *y*, −*z*), respectively.].

(3a*R*,4*R*,4'a*S*,5'*R*,7'*S*,7a*R*,9'*R*,9'a*S*)-5',9'-dihydroxy-7a-methyl-8'- methyleneperhydrospiro[isobenzofuran-4(1*H*),4'(3'H)- [1*H*-7,9a]methanocyclohepta[*c*]pyran]-1',3(3a*H*)-dione

Crystal data

$C_{20}H_{26}O_6$	F_{000} = 1552
M_r = 362.41	D_x = 1.340 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 2028 reflections
a = 12.2614 (15) Å	θ = 2.2–18.1º
b = 15.6668 (18) Å	μ = 0.10 mm^{-1}
c = 18.697 (2) Å	*T* = 298 (2) K
V = 3591.7 (8) Å^3	Prismatic, colorless
Z = 8	0.41 × 0.30 × 0.28 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3556 independent reflections
Radiation source: fine-focus sealed tube	1970 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.084
T = 298(2) K	θ_{max} = 25.0º

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 1999)

T_{min} = 0.961, T_{max} = 0.973

17440 measured reflections

θ_{min} = 1.7º

h = −13→14

k = −16→18

l = −22→18

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.078

$wR(F^2)$ = 0.237

S = 1.10

3556 reflections

472 parameters

1896 restraints

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

$w = 1/[\sigma^2(F_o^2) + (0.1062P)^2 + 2.5318P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max}$ = 0.54 e Å^{-3}

$\Delta\rho_{min}$ = −0.56 e Å^{-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 $F^2 > 2$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	0.3555 (6)	0.3465 (4)	−0.0342 (3)	0.0854 (18)
O1A	0.1460 (6)	0.4505 (4)	0.0174 (3)	0.0770 (16)
O2	0.2908 (4)	0.4019 (4)	0.1997 (3)	0.0642 (14)
O2A	0.2089 (4)	0.7286 (3)	0.0555 (3)	0.0599 (13)
O3	0.2473 (5)	0.5342 (4)	0.2199 (4)	0.089 (2)
O3A	0.2729 (4)	0.7432 (4)	0.1633 (3)	0.0644 (15)
O4	0.4497 (6)	0.6058 (3)	0.1203 (3)	0.0697 (16)
H4	0.4029	0.6414	0.1108	0.105*
O4A	0.0623 (5)	0.6303 (4)	0.2404 (3)	0.0615 (15)
H4A	0.1224	0.6081	0.2357	0.092*
O5	0.5642 (5)	0.3563 (4)	0.2942 (3)	0.0704 (16)

H5	0.6109	0.3235	0.3092	0.106*
O5A	−0.0730 (4)	0.8390 (3)	0.0395 (3)	0.0554 (14)
H5B	−0.1236	0.8706	0.0284	0.083*
O6	0.2848 (6)	0.2872 (5)	0.0616 (4)	0.105 (2)
O6A	0.2237 (5)	0.5683 (4)	−0.0221 (4)	0.0778 (18)
C1	0.3744 (7)	0.3381 (5)	0.1955 (5)	0.0627 (19)
H1A	0.3433	0.2858	0.1767	0.075*
H1B	0.4017	0.3263	0.2432	0.075*
C1A	0.1156 (6)	0.7223 (5)	0.0093 (4)	0.0555 (18)
H1C	0.1384	0.6989	−0.0364	0.067*
H1D	0.0868	0.7791	0.0007	0.067*
C3	0.3182 (7)	0.4818 (6)	0.2136 (4)	0.0581 (19)
C3A	0.1937 (7)	0.7400 (5)	0.1253 (5)	0.0496 (17)
C4	0.4375 (6)	0.5041 (5)	0.2221 (4)	0.0453 (16)
C4A	0.0797 (6)	0.7523 (5)	0.1533 (4)	0.0445 (15)
C5	0.4566 (7)	0.5961 (5)	0.1943 (4)	0.0566 (18)
H5A	0.4037	0.6343	0.2170	0.068*
C5A	0.0716 (7)	0.7189 (5)	0.2313 (4)	0.0545 (17)
H5C	0.1354	0.7390	0.2581	0.065*
C6	0.5690 (7)	0.6152 (5)	0.2241 (4)	0.0558 (18)
C6A	−0.0275 (7)	0.7649 (5)	0.2585 (4)	0.0578 (19)
C7	0.5801 (8)	0.5631 (5)	0.2931 (4)	0.0617 (19)
H7	0.5992	0.5991	0.3341	0.074*
C7A	−0.0466 (7)	0.8426 (5)	0.2124 (4)	0.0601 (19)
H7A	−0.0576	0.8938	0.2416	0.072*
C8	0.6638 (7)	0.4907 (5)	0.2817 (4)	0.0592 (19)
H8A	0.7243	0.5119	0.2534	0.071*
H8B	0.6923	0.4726	0.3277	0.071*
C8A	−0.1419 (6)	0.8280 (5)	0.1616 (4)	0.0501 (17)
H8C	−0.1726	0.8828	0.1482	0.060*
H8D	−0.1981	0.7959	0.1862	0.060*
C9	0.6122 (6)	0.4138 (5)	0.2436 (4)	0.0544 (18)
H9	0.6700	0.3832	0.2180	0.065*
C9A	−0.1089 (6)	0.7800 (5)	0.0939 (4)	0.0451 (16)
H9A	−0.1730	0.7494	0.0758	0.054*
C10	0.5252 (6)	0.4415 (4)	0.1887 (4)	0.0416 (15)
H10	0.5641	0.4747	0.1523	0.050*
C10A	−0.0175 (5)	0.7145 (4)	0.1078 (3)	0.0364 (14)
H10A	−0.0504	0.6702	0.1380	0.044*
C11	0.4689 (6)	0.3660 (5)	0.1479 (4)	0.0481 (16)
C11A	0.0259 (6)	0.6667 (4)	0.0400 (4)	0.0415 (14)
C12	0.5449 (7)	0.2881 (5)	0.1368 (5)	0.0625 (19)
H12A	0.5762	0.2723	0.1826	0.075*
H12B	0.5016	0.2403	0.1202	0.075*
C12A	−0.0584 (6)	0.6565 (5)	−0.0210 (4)	0.0505 (17)
H12C	−0.0933	0.7112	−0.0293	0.061*
H12D	−0.0203	0.6407	−0.0645	0.061*
C13	0.6370 (7)	0.3038 (6)	0.0839 (5)	0.068 (2)
H13A	0.6829	0.3500	0.1007	0.082*

H13B	0.6816	0.2529	0.0797	0.082*
C13A	−0.1465 (7)	0.5897 (5)	−0.0059 (4)	0.0597 (19)
H13C	−0.1879	0.6060	0.0362	0.072*
H13D	−0.1963	0.5863	−0.0461	0.072*
C14	0.5892 (7)	0.3265 (6)	0.0117 (5)	0.073 (2)
H14A	0.5464	0.2786	−0.0056	0.088*
H14B	0.6482	0.3358	−0.0219	0.088*
C14A	−0.0931 (7)	0.5037 (5)	0.0062 (5)	0.063 (2)
H14C	−0.0528	0.4877	−0.0364	0.076*
H14D	−0.1492	0.4611	0.0141	0.076*
C15	0.5169 (7)	0.4059 (5)	0.0133 (4)	0.0534 (18)
C15A	−0.0155 (6)	0.5047 (5)	0.0704 (4)	0.0508 (17)
C16	0.4396 (8)	0.4081 (6)	−0.0503 (4)	0.074 (2)
H16A	0.4085	0.4647	−0.0560	0.089*
H16B	0.4776	0.3928	−0.0939	0.089*
C16A	0.0601 (8)	0.4272 (5)	0.0665 (5)	0.070 (2)
H16C	0.0899	0.4143	0.1134	0.084*
H16D	0.0208	0.3776	0.0492	0.084*
C18	0.3476 (8)	0.3369 (7)	0.0369 (5)	0.072 (2)
C18A	0.1552 (8)	0.5350 (6)	0.0136 (5)	0.0597 (19)
C19	0.4297 (6)	0.3962 (5)	0.0736 (4)	0.0485 (16)
H19	0.3944	0.4518	0.0799	0.058*
C19A	0.0699 (6)	0.5773 (4)	0.0622 (4)	0.0431 (15)
H19A	0.1043	0.5845	0.1092	0.052*
C20	0.4656 (7)	0.5224 (5)	0.3016 (4)	0.0589 (18)
H20A	0.4142	0.5619	0.3231	0.071*
H20B	0.4683	0.4704	0.3297	0.071*
C20A	0.0601 (7)	0.8482 (5)	0.1686 (4)	0.0578 (18)
H20C	0.1190	0.8730	0.1963	0.069*
H20D	0.0502	0.8806	0.1248	0.069*
C21	0.6457 (8)	0.6594 (6)	0.1925 (6)	0.081 (3)
H21A	0.6335	0.6825	0.1474	0.098*
H21B	0.7123	0.6677	0.2152	0.098*
C21A	−0.0921 (8)	0.7372 (7)	0.3096 (5)	0.091 (3)
H21C	−0.0777	0.6854	0.3319	0.109*
H21D	−0.1521	0.7695	0.3234	0.109*
C22	0.5889 (7)	0.4864 (6)	0.0139 (5)	0.065 (2)
H22A	0.6405	0.4827	0.0524	0.098*
H22B	0.5439	0.5360	0.0204	0.098*
H22C	0.6273	0.4908	−0.0307	0.098*
C22A	−0.0819 (8)	0.5005 (5)	0.1404 (4)	0.066 (2)
H22D	−0.1183	0.4464	0.1434	0.099*
H22E	−0.1350	0.5455	0.1408	0.099*
H22F	−0.0337	0.5069	0.1805	0.099*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

O1	0.076 (4)	0.102 (4)	0.077 (4)	−0.006 (4)	−0.011 (3)	−0.034 (3)
O1A	0.081 (4)	0.056 (3)	0.094 (4)	0.013 (3)	−0.034 (3)	0.002 (3)
O2	0.045 (3)	0.069 (3)	0.079 (3)	0.006 (3)	0.008 (3)	0.010 (3)
O2A	0.038 (3)	0.070 (3)	0.072 (3)	−0.011 (2)	−0.007 (3)	−0.002 (3)
O3	0.057 (4)	0.091 (4)	0.118 (5)	0.034 (4)	0.006 (4)	−0.002 (4)
O3A	0.033 (3)	0.067 (4)	0.094 (4)	−0.005 (3)	0.015 (3)	−0.004 (3)
O4	0.097 (4)	0.061 (3)	0.052 (3)	0.015 (3)	−0.010 (3)	0.012 (3)
O4A	0.059 (3)	0.073 (4)	0.053 (3)	0.020 (3)	−0.004 (3)	−0.010 (3)
O5	0.064 (3)	0.077 (4)	0.070 (3)	0.021 (3)	0.003 (3)	0.031 (3)
O5A	0.055 (3)	0.056 (3)	0.056 (3)	0.006 (3)	−0.006 (3)	−0.017 (3)
O6	0.092 (5)	0.104 (5)	0.119 (5)	−0.047 (4)	−0.003 (4)	−0.014 (4)
O6A	0.060 (4)	0.080 (4)	0.093 (4)	0.002 (3)	−0.037 (4)	0.000 (3)
C1	0.059 (4)	0.054 (4)	0.074 (4)	−0.005 (4)	0.010 (4)	0.009 (4)
C1A	0.049 (4)	0.061 (4)	0.057 (4)	0.005 (3)	−0.008 (3)	−0.008 (3)
C3	0.064 (4)	0.059 (4)	0.051 (4)	0.010 (4)	0.006 (4)	0.010 (3)
C3A	0.042 (4)	0.041 (4)	0.065 (4)	−0.004 (3)	0.005 (3)	−0.002 (3)
C4	0.042 (3)	0.047 (3)	0.047 (3)	0.005 (3)	0.006 (3)	0.001 (3)
C4A	0.038 (3)	0.050 (3)	0.045 (3)	0.004 (3)	0.007 (3)	0.004 (3)
C5	0.070 (4)	0.049 (4)	0.051 (4)	0.018 (3)	−0.005 (4)	−0.003 (3)
C5A	0.047 (3)	0.066 (4)	0.051 (4)	0.015 (3)	0.011 (3)	0.009 (3)
C6	0.067 (4)	0.044 (4)	0.057 (4)	0.009 (4)	−0.002 (4)	−0.009 (3)
C6A	0.056 (4)	0.075 (4)	0.042 (4)	0.012 (4)	0.014 (4)	0.011 (3)
C7	0.080 (4)	0.062 (4)	0.043 (4)	0.003 (4)	−0.004 (4)	−0.013 (3)
C7A	0.058 (4)	0.063 (4)	0.059 (4)	0.012 (4)	0.011 (4)	0.022 (3)
C8	0.050 (4)	0.073 (4)	0.055 (4)	0.008 (4)	−0.007 (4)	0.005 (4)
C8A	0.041 (4)	0.056 (4)	0.053 (4)	0.008 (3)	0.001 (3)	−0.006 (3)
C9	0.049 (4)	0.056 (4)	0.058 (4)	0.014 (3)	0.008 (3)	0.007 (3)
C9A	0.041 (3)	0.046 (4)	0.048 (3)	−0.002 (3)	0.001 (3)	−0.004 (3)
C10	0.040 (3)	0.041 (3)	0.044 (3)	0.010 (3)	0.003 (3)	0.008 (3)
C10A	0.029 (3)	0.041 (3)	0.039 (3)	−0.003 (3)	−0.001 (3)	−0.004 (3)
C11	0.042 (3)	0.042 (3)	0.060 (3)	0.006 (3)	0.010 (3)	0.000 (3)
C11A	0.034 (3)	0.045 (3)	0.045 (3)	−0.007 (3)	−0.003 (3)	−0.004 (3)
C12	0.066 (4)	0.045 (4)	0.076 (4)	0.008 (4)	0.004 (4)	−0.003 (3)
C12A	0.050 (4)	0.062 (4)	0.039 (3)	0.002 (3)	0.002 (3)	0.000 (3)
C13	0.057 (4)	0.066 (4)	0.082 (5)	0.023 (4)	0.009 (4)	−0.005 (4)
C13A	0.053 (4)	0.071 (4)	0.055 (4)	−0.004 (4)	0.008 (4)	0.008 (4)
C14	0.063 (4)	0.081 (5)	0.077 (4)	0.005 (4)	0.009 (4)	−0.021 (4)
C14A	0.063 (4)	0.058 (4)	0.068 (4)	−0.012 (4)	−0.008 (4)	0.009 (4)
C15	0.051 (4)	0.061 (4)	0.047 (4)	0.010 (3)	0.004 (3)	−0.010 (3)
C15A	0.052 (4)	0.043 (4)	0.057 (4)	0.004 (3)	−0.011 (3)	−0.001 (3)
C16	0.066 (5)	0.098 (5)	0.057 (4)	0.015 (5)	0.005 (4)	−0.016 (4)
C16A	0.072 (5)	0.050 (4)	0.089 (5)	0.001 (4)	−0.024 (4)	−0.004 (4)
C18	0.060 (4)	0.078 (4)	0.078 (4)	0.003 (4)	−0.002 (4)	−0.009 (4)
C18A	0.053 (4)	0.061 (4)	0.065 (4)	0.010 (4)	−0.006 (4)	−0.001 (4)
C19	0.043 (3)	0.047 (3)	0.055 (3)	−0.005 (3)	0.002 (3)	−0.008 (3)
C19A	0.037 (3)	0.051 (3)	0.041 (3)	0.000 (3)	−0.005 (3)	0.001 (3)
C20	0.069 (4)	0.061 (4)	0.046 (3)	0.027 (3)	0.009 (3)	0.002 (3)
C20A	0.052 (4)	0.053 (4)	0.069 (4)	−0.002 (3)	0.013 (3)	0.008 (3)
C21	0.088 (6)	0.069 (6)	0.087 (6)	−0.019 (5)	−0.007 (6)	−0.003 (5)

C21A	0.090 (6)	0.123 (7)	0.059 (5)	0.054 (6)	−0.012 (5)	−0.023 (5)
C22	0.059 (5)	0.075 (5)	0.061 (5)	−0.005 (4)	0.012 (4)	0.007 (4)
C22A	0.069 (5)	0.061 (5)	0.069 (5)	−0.004 (4)	−0.022 (4)	−0.009 (4)

Geometric parameters (Å, °)

O1—C18	1.343 (11)	C9A—C10A	1.543 (9)
O1—C16	1.444 (11)	C9A—H9A	0.9800
O1A—C18A	1.330 (10)	C10—C11	1.568 (10)
O1A—C16A	1.445 (11)	C10—H10	0.9800
O2—C3	1.323 (10)	C10A—C11A	1.566 (9)
O2—C1	1.432 (10)	C10A—H10A	0.9800
O2A—C3A	1.330 (9)	C11—C19	1.544 (10)
O2A—C1A	1.438 (9)	C11—C12	1.549 (10)
O3—C3	1.201 (10)	C11A—C12A	1.548 (10)
O3A—C3A	1.204 (9)	C11A—C19A	1.556 (10)
O4—C5	1.394 (9)	C12—C13	1.522 (12)
O4—H4	0.8200	C12—H12A	0.9700
O4A—C5A	1.404 (9)	C12—H12B	0.9700
O4A—H4A	0.8200	C12A—C13A	1.530 (11)
O5—C9	1.433 (9)	C12A—H12C	0.9700
O5—H5	0.8200	C12A—H12D	0.9700
O5A—C9A	1.443 (8)	C13—C14	1.515 (12)
O5A—H5B	0.8200	C13—H13A	0.9700
O6—C18	1.188 (11)	C13—H13B	0.9700
O6A—C18A	1.192 (10)	C13A—C14A	1.515 (11)
C1—C11	1.526 (10)	C13A—H13C	0.9700
C1—H1A	0.9700	C13A—H13D	0.9700
C1—H1B	0.9700	C14—C15	1.528 (11)
C1A—C11A	1.516 (10)	C14—H14A	0.9700
C1A—H1C	0.9700	C14—H14B	0.9700
C1A—H1D	0.9700	C14A—C15A	1.532 (11)
C3—C4	1.512 (12)	C14A—H14C	0.9700
C3A—C4A	1.504 (10)	C14A—H14D	0.9700
C4—C5	1.551 (11)	C15—C16	1.521 (11)
C4—C20	1.553 (10)	C15—C22	1.539 (11)
C4—C10	1.584 (10)	C15—C19	1.561 (10)
C4A—C20A	1.548 (11)	C15A—C16A	1.529 (11)
C4A—C5A	1.554 (10)	C15A—C22A	1.542 (11)
C4A—C10A	1.579 (10)	C15A—C19A	1.554 (10)
C5—C6	1.516 (12)	C16—H16A	0.9700
C5—H5A	0.9800	C16—H16B	0.9700
C5A—C6A	1.501 (11)	C16A—H16C	0.9700
C5A—H5C	0.9800	C16A—H16D	0.9700
C6—C21	1.308 (12)	C18—C19	1.531 (12)
C6—C7	1.533 (11)	C18A—C19A	1.537 (11)
C6A—C21A	1.314 (12)	C19—H19	0.9800
C6A—C7A	1.510 (11)	C19A—H19A	0.9800
C7—C8	1.544 (11)	C20—H20A	0.9700

C7—C20	1.550 (12)	C20—H20B	0.9700
C7—H7	0.9800	C20A—H20C	0.9700
C7A—C8A	1.523 (11)	C20A—H20D	0.9700
C7A—C20A	1.546 (11)	C21—H21A	0.9300
C7A—H7A	0.9800	C21—H21B	0.9300
C8—C9	1.536 (11)	C21A—H21C	0.9300
C8—H8A	0.9700	C21A—H21D	0.9300
C8—H8B	0.9700	C22—H22A	0.9600
C8A—C9A	1.527 (10)	C22—H22B	0.9600
C8A—H8C	0.9700	C22—H22C	0.9600
C8A—H8D	0.9700	C22A—H22D	0.9600
C9—C10	1.543 (10)	C22A—H22E	0.9600
C9—H9	0.9800	C22A—H22F	0.9600
C18—O1—C16	109.4 (7)	C12A—C11A—C19A	109.6 (6)
C18A—O1A—C16A	110.4 (7)	C1A—C11A—C10A	106.2 (6)
C3—O2—C1	119.3 (7)	C12A—C11A—C10A	114.8 (6)
C3A—O2A—C1A	119.2 (6)	C19A—C11A—C10A	109.3 (5)
C5—O4—H4	109.5	C13—C12—C11	114.0 (7)
C5A—O4A—H4A	109.5	C13—C12—H12A	108.8
C9—O5—H5	109.5	C11—C12—H12A	108.8
C9A—O5A—H5B	109.5	C13—C12—H12B	108.8
O2—C1—C11	112.1 (6)	C11—C12—H12B	108.8
O2—C1—H1A	109.2	H12A—C12—H12B	107.7
C11—C1—H1A	109.2	C13A—C12A—C11A	114.0 (6)
O2—C1—H1B	109.2	C13A—C12A—H12C	108.8
C11—C1—H1B	109.2	C11A—C12A—H12C	108.8
H1A—C1—H1B	107.9	C13A—C12A—H12D	108.8
O2A—C1A—C11A	112.9 (6)	C11A—C12A—H12D	108.8
O2A—C1A—H1C	109.0	H12C—C12A—H12D	107.7
C11A—C1A—H1C	109.0	C14—C13—C12	109.3 (7)
O2A—C1A—H1D	109.0	C14—C13—H13A	109.8
C11A—C1A—H1D	109.0	C12—C13—H13A	109.8
H1C—C1A—H1D	107.8	C14—C13—H13B	109.8
O3—C3—O2	118.9 (8)	C12—C13—H13B	109.8
O3—C3—C4	122.1 (8)	H13A—C13—H13B	108.3
O2—C3—C4	119.0 (7)	C14A—C13A—C12A	109.3 (7)
O3A—C3A—O2A	118.1 (7)	C14A—C13A—H13C	109.8
O3A—C3A—C4A	122.6 (7)	C12A—C13A—H13C	109.8
O2A—C3A—C4A	119.2 (7)	C14A—C13A—H13D	109.8
C3—C4—C5	109.0 (6)	C12A—C13A—H13D	109.8
C3—C4—C20	111.0 (6)	H13C—C13A—H13D	108.3
C5—C4—C20	96.6 (6)	C13—C14—C15	113.4 (7)
C3—C4—C10	118.2 (7)	C13—C14—H14A	108.9
C5—C4—C10	109.9 (6)	C15—C14—H14A	108.9
C20—C4—C10	110.0 (6)	C13—C14—H14B	108.9
C3A—C4A—C20A	109.5 (6)	C15—C14—H14B	108.9
C3A—C4A—C5A	110.0 (6)	H14A—C14—H14B	107.7
C20A—C4A—C5A	98.2 (6)	C13A—C14A—C15A	112.1 (7)
C3A—C4A—C10A	117.8 (6)	C13A—C14A—H14C	109.2

C20A—C4A—C10A	110.3 (6)	C15A—C14A—H14C	109.2
C5A—C4A—C10A	109.3 (6)	C13A—C14A—H14D	109.2
O4—C5—C6	113.5 (7)	C15A—C14A—H14D	109.2
O4—C5—C4	115.1 (6)	H14C—C14A—H14D	107.9
C6—C5—C4	101.4 (6)	C16—C15—C14	111.3 (7)
O4—C5—H5A	108.8	C16—C15—C22	110.1 (7)
C6—C5—H5A	108.8	C14—C15—C22	109.6 (7)
C4—C5—H5A	108.8	C16—C15—C19	98.0 (6)
O4A—C5A—C6A	111.6 (7)	C14—C15—C19	109.4 (7)
O4A—C5A—C4A	116.8 (6)	C22—C15—C19	117.9 (6)
C6A—C5A—C4A	102.0 (6)	C16A—C15A—C14A	109.4 (7)
O4A—C5A—H5C	108.7	C16A—C15A—C22A	109.0 (7)
C6A—C5A—H5C	108.7	C14A—C15A—C22A	109.7 (7)
C4A—C5A—H5C	108.7	C16A—C15A—C19A	99.7 (6)
C21—C6—C5	126.3 (8)	C14A—C15A—C19A	110.4 (6)
C21—C6—C7	126.7 (8)	C22A—C15A—C19A	118.1 (6)
C5—C6—C7	106.6 (7)	O1—C16—C15	105.5 (7)
C21A—C6A—C5A	125.1 (8)	O1—C16—H16A	110.6
C21A—C6A—C7A	126.0 (8)	C15—C16—H16A	110.6
C5A—C6A—C7A	108.6 (6)	O1—C16—H16B	110.6
C6—C7—C8	109.5 (6)	C15—C16—H16B	110.6
C6—C7—C20	103.0 (7)	H16A—C16—H16B	108.8
C8—C7—C20	108.3 (6)	O1A—C16A—C15A	105.8 (7)
C6—C7—H7	111.9	O1A—C16A—H16C	110.6
C8—C7—H7	111.9	C15A—C16A—H16C	110.6
C20—C7—H7	111.9	O1A—C16A—H16D	110.6
C6A—C7A—C8A	110.8 (7)	C15A—C16A—H16D	110.6
C6A—C7A—C20A	102.6 (6)	H16C—C16A—H16D	108.7
C8A—C7A—C20A	109.1 (6)	O6—C18—O1	120.3 (10)
C6A—C7A—H7A	111.4	O6—C18—C19	130.6 (9)
C8A—C7A—H7A	111.4	O1—C18—C19	109.2 (8)
C20A—C7A—H7A	111.4	O6A—C18A—O1A	121.7 (9)
C9—C8—C7	111.5 (7)	O6A—C18A—C19A	128.5 (8)
C9—C8—H8A	109.3	O1A—C18A—C19A	109.8 (8)
C7—C8—H8A	109.3	C18—C19—C11	114.9 (7)
C9—C8—H8B	109.3	C18—C19—C15	100.8 (6)
C7—C8—H8B	109.3	C11—C19—C15	117.7 (6)
H8A—C8—H8B	108.0	C18—C19—H19	107.6
C7A—C8A—C9A	112.8 (6)	C11—C19—H19	107.6
C7A—C8A—H8C	109.0	C15—C19—H19	107.6
C9A—C8A—H8C	109.0	C18A—C19A—C15A	101.6 (6)
C7A—C8A—H8D	109.0	C18A—C19A—C11A	117.7 (6)
C9A—C8A—H8D	109.0	C15A—C19A—C11A	116.8 (6)
H8C—C8A—H8D	107.8	C18A—C19A—H19A	106.6
O5—C9—C8	110.8 (6)	C15A—C19A—H19A	106.6
O5—C9—C10	109.4 (6)	C11A—C19A—H19A	106.6
C8—C9—C10	111.9 (6)	C7—C20—C4	100.3 (6)
O5—C9—H9	108.2	C7—C20—H20A	111.7
C8—C9—H9	108.2	C4—C20—H20A	111.7

C10—C9—H9	108.2	C7—C20—H20B	111.7
O5A—C9A—C8A	110.4 (6)	C4—C20—H20B	111.7
O5A—C9A—C10A	108.9 (5)	H20A—C20—H20B	109.5
C8A—C9A—C10A	112.4 (6)	C7A—C20A—C4A	100.0 (6)
O5A—C9A—H9A	108.4	C7A—C20A—H20C	111.8
C8A—C9A—H9A	108.4	C4A—C20A—H20C	111.8
C10A—C9A—H9A	108.4	C7A—C20A—H20D	111.8
C9—C10—C11	114.6 (6)	C4A—C20A—H20D	111.8
C9—C10—C4	112.4 (6)	H20C—C20A—H20D	109.5
C11—C10—C4	111.1 (6)	C6—C21—H21A	120.0
C9—C10—H10	106.0	C6—C21—H21B	120.0
C11—C10—H10	106.0	H21A—C21—H21B	120.0
C4—C10—H10	106.0	C6A—C21A—H21C	120.0
C9A—C10A—C11A	115.3 (5)	C6A—C21A—H21D	120.0
C9A—C10A—C4A	112.9 (5)	H21C—C21A—H21D	120.0
C11A—C10A—C4A	111.1 (5)	C15—C22—H22A	109.5
C9A—C10A—H10A	105.5	C15—C22—H22B	109.5
C11A—C10A—H10A	105.5	H22A—C22—H22B	109.5
C4A—C10A—H10A	105.5	C15—C22—H22C	109.5
C1—C11—C19	112.1 (6)	H22A—C22—H22C	109.5
C1—C11—C12	108.0 (6)	H22B—C22—H22C	109.5
C19—C11—C12	108.0 (6)	C15A—C22A—H22D	109.5
C1—C11—C10	105.5 (6)	C15A—C22A—H22E	109.5
C19—C11—C10	110.1 (6)	H22D—C22A—H22E	109.5
C12—C11—C10	113.2 (6)	C15A—C22A—H22F	109.5
C1A—C11A—C12A	105.4 (6)	H22D—C22A—H22F	109.5
C1A—C11A—C19A	111.5 (6)	H22E—C22A—H22F	109.5
C3—O2—C1—C11	−48.6 (10)	C9—C10—C11—C12	−31.4 (9)
C3A—O2A—C1A—C11A	−43.2 (9)	C4—C10—C11—C12	−160.1 (6)
C1—O2—C3—O3	−177.0 (7)	O2A—C1A—C11A—C12A	−171.7 (6)
C1—O2—C3—C4	2.0 (10)	O2A—C1A—C11A—C19A	−52.9 (8)
C1A—O2A—C3A—O3A	178.3 (7)	O2A—C1A—C11A—C10A	66.1 (8)
C1A—O2A—C3A—C4A	−4.4 (10)	C9A—C10A—C11A—C1A	87.5 (7)
O3—C3—C4—C5	−33.7 (10)	C4A—C10A—C11A—C1A	−42.6 (7)
O2—C3—C4—C5	147.3 (7)	C9A—C10A—C11A—C12A	−28.5 (8)
O3—C3—C4—C20	71.5 (10)	C4A—C10A—C11A—C12A	−158.6 (6)
O2—C3—C4—C20	−107.5 (8)	C9A—C10A—C11A—C19A	−152.1 (6)
O3—C3—C4—C10	−160.1 (7)	C4A—C10A—C11A—C19A	77.8 (7)
O2—C3—C4—C10	21.0 (10)	C1—C11—C12—C13	173.9 (7)
O3A—C3A—C4A—C20A	75.2 (9)	C19—C11—C12—C13	52.5 (9)
O2A—C3A—C4A—C20A	−102.0 (8)	C10—C11—C12—C13	−69.7 (9)
O3A—C3A—C4A—C5A	−31.7 (10)	C1A—C11A—C12A—C13A	169.9 (6)
O2A—C3A—C4A—C5A	151.2 (7)	C19A—C11A—C12A—C13A	49.8 (8)
O3A—C3A—C4A—C10A	−157.8 (7)	C10A—C11A—C12A—C13A	−73.7 (8)
O2A—C3A—C4A—C10A	25.1 (10)	C11—C12—C13—C14	−59.8 (10)
C3—C4—C5—O4	−71.1 (9)	C11A—C12A—C13A—C14A	−59.2 (9)
C20—C4—C5—O4	174.0 (7)	C12—C13—C14—C15	59.2 (10)
C10—C4—C5—O4	59.9 (9)	C12A—C13A—C14A—C15A	60.9 (9)
C3—C4—C5—C6	165.9 (6)	C13—C14—C15—C16	−159.2 (8)

C20—C4—C5—C6	51.0 (7)	C13—C14—C15—C22	78.7 (9)
C10—C4—C5—C6	−63.1 (7)	C13—C14—C15—C19	−52.0 (9)
C3A—C4A—C5A—O4A	−78.8 (9)	C13A—C14A—C15A—C16A	−163.1 (7)
C20A—C4A—C5A—O4A	167.0 (6)	C13A—C14A—C15A—C22A	77.4 (8)
C10A—C4A—C5A—O4A	52.0 (8)	C13A—C14A—C15A—C19A	−54.4 (9)
C3A—C4A—C5A—C6A	159.4 (6)	C18—O1—C16—C15	25.3 (9)
C20A—C4A—C5A—C6A	45.1 (8)	C14—C15—C16—O1	75.6 (8)
C10A—C4A—C5A—C6A	−69.9 (7)	C22—C15—C16—O1	−162.7 (6)
O4—C5—C6—C21	19.4 (12)	C19—C15—C16—O1	−39.0 (8)
C4—C5—C6—C21	143.5 (9)	C18A—O1A—C16A—C15A	23.0 (9)
O4—C5—C6—C7	−153.2 (6)	C14A—C15A—C16A—O1A	81.6 (8)
C4—C5—C6—C7	−29.1 (7)	C22A—C15A—C16A—O1A	−158.5 (6)
O4A—C5A—C6A—C21A	27.6 (12)	C19A—C15A—C16A—O1A	−34.2 (7)
C4A—C5A—C6A—C21A	153.0 (9)	C16—O1—C18—O6	−178.1 (9)
O4A—C5A—C6A—C7A	−146.7 (7)	C16—O1—C18—C19	1.0 (10)
C4A—C5A—C6A—C7A	−21.2 (9)	C16A—O1A—C18A—O6A	177.5 (8)
C21—C6—C7—C8	−62.3 (11)	C16A—O1A—C18A—C19A	−0.6 (9)
C5—C6—C7—C8	110.3 (7)	O6—C18—C19—C11	25.6 (14)
C21—C6—C7—C20	−177.4 (8)	O1—C18—C19—C11	−153.3 (7)
C5—C6—C7—C20	−4.9 (8)	O6—C18—C19—C15	153.3 (11)
C21A—C6A—C7A—C8A	−69.4 (11)	O1—C18—C19—C15	−25.6 (9)
C5A—C6A—C7A—C8A	104.7 (7)	C1—C11—C19—C18	−47.2 (9)
C21A—C6A—C7A—C20A	174.3 (9)	C12—C11—C19—C18	71.6 (8)
C5A—C6A—C7A—C20A	−11.5 (9)	C10—C11—C19—C18	−164.3 (6)
C6—C7—C8—C9	−81.4 (8)	C1—C11—C19—C15	−165.8 (6)
C20—C7—C8—C9	30.3 (9)	C12—C11—C19—C15	−46.9 (9)
C6A—C7A—C8A—C9A	−83.1 (8)	C10—C11—C19—C15	77.2 (8)
C20A—C7A—C8A—C9A	29.0 (9)	C16—C15—C19—C18	37.5 (8)
C7—C8—C9—O5	−87.8 (7)	C14—C15—C19—C18	−78.5 (8)
C7—C8—C9—C10	34.6 (9)	C22—C15—C19—C18	155.4 (7)
C7A—C8A—C9A—O5A	−88.3 (7)	C16—C15—C19—C11	163.3 (7)
C7A—C8A—C9A—C10A	33.5 (9)	C14—C15—C19—C11	47.3 (9)
O5—C9—C10—C11	−56.6 (8)	C22—C15—C19—C11	−78.8 (9)
C8—C9—C10—C11	−179.8 (6)	O6A—C18A—C19A—C15A	160.9 (8)
O5—C9—C10—C4	71.4 (8)	O1A—C18A—C19A—C15A	−21.2 (8)
C8—C9—C10—C4	−51.8 (8)	O6A—C18A—C19A—C11A	32.0 (12)
C3—C4—C10—C9	−127.3 (7)	O1A—C18A—C19A—C11A	−150.1 (6)
C5—C4—C10—C9	106.8 (7)	C16A—C15A—C19A—C18A	32.2 (7)
C20—C4—C10—C9	1.6 (8)	C14A—C15A—C19A—C18A	−82.8 (7)
C3—C4—C10—C11	2.5 (9)	C22A—C15A—C19A—C18A	150.0 (7)
C5—C4—C10—C11	−123.4 (6)	C16A—C15A—C19A—C11A	161.7 (6)
C20—C4—C10—C11	131.5 (6)	C14A—C15A—C19A—C11A	46.7 (8)
O5A—C9A—C10A—C11A	−53.7 (7)	C22A—C15A—C19A—C11A	−80.5 (8)
C8A—C9A—C10A—C11A	−176.3 (6)	C1A—C11A—C19A—C18A	−38.9 (9)
O5A—C9A—C10A—C4A	75.5 (7)	C12A—C11A—C19A—C18A	77.4 (8)
C8A—C9A—C10A—C4A	−47.1 (8)	C10A—C11A—C19A—C18A	−156.0 (6)
C3A—C4A—C10A—C9A	−129.7 (7)	C1A—C11A—C19A—C15A	−160.3 (6)
C20A—C4A—C10A—C9A	−3.1 (8)	C12A—C11A—C19A—C15A	−44.0 (8)
C5A—C4A—C10A—C9A	103.9 (7)	C10A—C11A—C19A—C15A	82.7 (7)

C3A—C4A—C10A—C11A	1.6 (9)	C6—C7—C20—C4	36.9 (7)
C20A—C4A—C10A—C11A	128.3 (6)	C8—C7—C20—C4	−79.1 (7)
C5A—C4A—C10A—C11A	−124.8 (6)	C3—C4—C20—C7	−167.3 (6)
O2—C1—C11—C19	−52.1 (9)	C5—C4—C20—C7	−54.0 (7)
O2—C1—C11—C12	−170.9 (7)	C10—C4—C20—C7	59.9 (7)
O2—C1—C11—C10	67.8 (8)	C6A—C7A—C20A—C4A	39.8 (8)
C9—C10—C11—C1	86.4 (7)	C8A—C7A—C20A—C4A	−77.7 (7)
C4—C10—C11—C1	−42.3 (7)	C3A—C4A—C20A—C7A	−167.0 (6)
C9—C10—C11—C19	−152.5 (6)	C5A—C4A—C20A—C7A	−52.3 (7)
C4—C10—C11—C19	78.8 (7)	C10A—C4A—C20A—C7A	61.9 (7)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O3A	0.82	2.46	3.159 (8)	144
O4A—H4A···O3	0.82	1.94	2.750 (8)	168
O5—H5···O3A^{i}	0.82	1.97	2.787 (8)	175
O5A—H5B···O6A^{ii}	0.82	2.11	2.903 (9)	164

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) *x*−1/2, −*y*+3/2, −*z*.

Comparison of the puckering parameters (Å, °) for the six- and five-membered rings of molecules 1 and 2

Molecule	A			B		
Puckering parameters	Q	θ	φ	Q	θ	φ
Ring A, A"	0.545 (9)	171.2 (9)	296 (6)	0.546 (8)	168.9 (8)	315 (5)
Ring B, B"	0.584 (9)	65.6 (8)	91.8 (8)	0.582 (8)	68.4 (8)	95.2 (7)
Ring C, C"	0.861 (8)	80.2 (5)	286.4 (6)	0.837 (8)	78.9 (5)	288.8 (6)
Puckering parameters		Q2	φ2		Q2	φ2
Ring D, D"		0.561 (9)	174.6 (9)		0.530 (9)	167.1 (9)
Ring E, E"		0.412 (9)	254.0 (13)		0.355 (9)	251.8 (14)

Ring A: C11···C15-C19 Ring A": C11A···C15A-C19A Ring B: O2-C1-C11-C10-C4-C3 Ring B": O2A-C1A-C11A-C10A-C4A-C3A Ring C: C4-C10-C9-C8-C7-C20 Ring C": C4A-C10A-C9A-C8A-C7A-C20A Ring D: C4···C7-C20 Ring D": C4A···C7A-C20A Ring E: O1-C16-C15-C19-C18 Ring E": O1A-C16A-C15A-C19A-C18A

Fig. 1

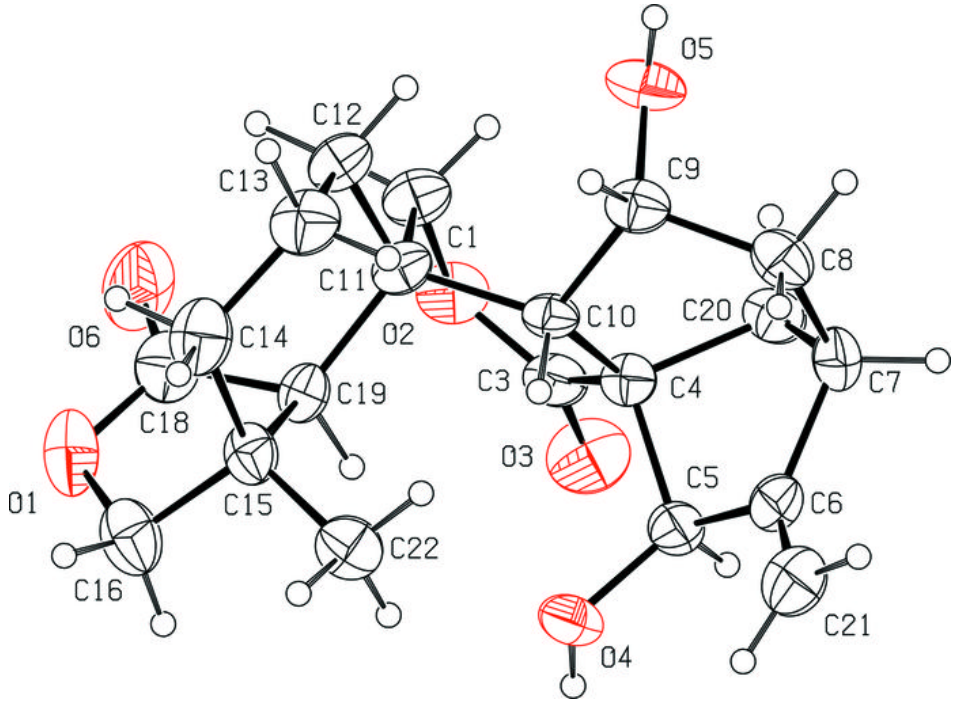
O5
C12
C13
C9
C1
C11
C8
O6
C14
O2
C10
C20
C3
C4
C7
C19
C18
O3
C5
O1
C15
C6
C22
C16
C21
O4

Fig. 2

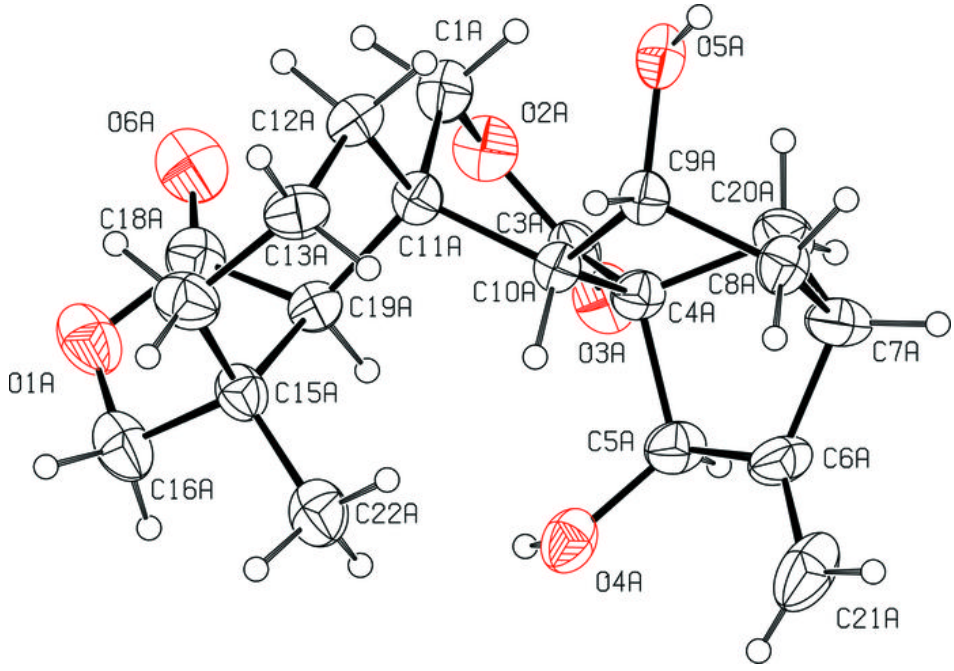
C1A
O5A
O6A
C12A
O2A
C9A
C20A
C18A
C3A
C13A
C11A
C10A
C8A
C4A
C19A
O3A
C7A
O1A
C15A
C5A
C6A
C16A
C22A
O4A
C21A

Fig. 3