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Arctigenin: a lignan from *Arctium lappa*

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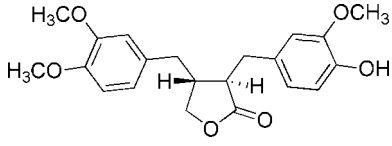
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.033; wR factor = 0.079; data-to-parameter ratio = 10.3.

The title compound {systematic name: (3*R-trans*)-4-[(3,4-dimethoxyphenyl)methyl]-3-[(4-hydroxy-3-methoxyphenyl)-methyl]-4,5-dihydrofuran-2(3*H*)-one}, $C_{21}H_{24}O_6$, has a dibenzylbutyrolactone skeleton. The two aromatic rings are inclined at a dihedral angle of 68.75 (7)° with respect to each other. The lactone ring adopts an envelope conformation. A series of O—H···O and C—H···O hydrogen bonds contribute to the stabilization of the crystal packing. The absolute configuration was assigned on the basis of the published literature.

Related literature

For related literature, see: Awale *et al.* (2006). For a similar structure, see: Bruno-Colmenárez *et al.* (2007).



Experimental

Crystal data

$C_{21}H_{24}O_6$
M_r = 372.40
Orthorhombic, $P2_12_12_1$
a = 9.4845 (19) Å
b = 10.065 (2) Å
c = 19.915 (4) Å
V = 1901.2 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 113 (2) K
0.14 × 0.12 × 0.10 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.987, T_{max} = 0.991
13910 measured reflections
2581 independent reflections
2449 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.079
S = 1.06
2581 reflections
251 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5···O2^{i}	0.90 (2)	2.04 (2)	2.8280 (17)	146 (2)
O5—H5···O6	0.90 (2)	2.22 (2)	2.6799 (18)	111.7 (17)
O5—H5···O1^{i}	0.90 (2)	2.58 (2)	3.2406 (18)	130.8 (16)
C3—H3···O5^{ii}	0.95	2.34	3.278 (2)	168
C14—H14*A*···O4^{iii}	0.99	2.86	3.687 (2)	142
C14—H14*B*···O5^{iv}	0.99	2.42	3.373 (2)	162
C20—H20···O4^{iii}	0.95	2.53	3.446 (2)	162

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2005).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2739).

References

Awale, S., Lu, J., Kalaumi, S. K., Kurashima, Y., Tezuka, Y., Kadaota, S. & Esumi, H. (2006). *Cancer Res.* **66**, 1751–1757.
Bruno-Colmenárez, J., Usubillaga, A., Khouri, N. & Díaz de Delgado, G. (2007). *Acta Cryst.* E**63**, o2046–o2047.
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supplementary materials

Acta Cryst. (2008). E**64**, o1538 [**doi:10.1107/S1600536808021752**]

Arctigenin: a lignan from *Arctium lappa*

H. Gao, G. Li, J. Zhang and J. Zeng

Comment

Arctigenin has been identified as an antitumor agent with the ability to eliminate the tolerance of cancer cells to nutrient strarvation (Awale *et al.*, 2006).

The title compound has a dibenzylbutyrolactone skeleton (Fig. 1). The two aromatic rings have a dihedral angle of 68.75 (7)°. The lactone ring adopts an envelope conformation. A series of O—H···O and C—H···O hydrogen bonds contribute to the stabilization of the crystal packing (Table 1).

Experimental

Arctigenin was isolated from Chinese medicine Arctium lappa. Crystal blocks were obtained by natural evaporation of a methanolic solution.

Refinement

In the absence of anomalous scatterers Friedel pairs were merged. The absolute configuration was set according to the literature (Awale *et al.*, 2006). The O-bound H atom was located in a difference map and freely refined. All other H atoms were positioned geometrically and refined as riding atoms, with U(H) = 1.2 U_{eq}(CH and CH_2) and C—H ranging from 0.95–1.0Å or U(H) = 1.5 U_{eq}(CH_3) and C_{methyl}—H =0.99 Å. The methyl groups were allowed to rotate but not to tip.

Figures

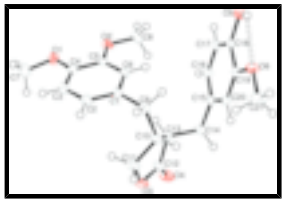


Fig. 1. The molecular structure of (I) with the atom-numbering scheme and 50% probability displacement ellipsoids.

(3R-trans)-4-[(3,4-dimethoxyphenyl)methyl]-3-[(4-hydroxy- 3-methoxyphenyl)methyl]-4,5-dihydrofuran-2(3H)-one

Crystal data

$C_{21}H_{24}O_6$	F_{000} = 792
M_r = 372.40	D_x = 1.301 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å

Hall symbol: P 2ac 2ab	Cell parameters from 5995 reflections
a = 9.4845 (19) Å	θ = 2.3–27.9º
b = 10.065 (2) Å	μ = 0.10 mm^{-1}
c = 19.915 (4) Å	T = 113 (2) K
V = 1901.2 (7) $Å^3$	Block, colourless
Z = 4	0.14 × 0.12 × 0.10 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer	2581 independent reflections
Radiation source: rotating anode	2449 reflections with $I > 2\sigma(I)$
Monochromator: confocal	R_{int} = 0.037
Detector resolution: 7.31 pixels mm^{-1}	θ_{max} = 27.8º
T = 113(2) K	θ_{min} = 2.1º
ω scans	h = −12→12
Absorption correction: multi-scan (CrystalClear; Rigaku/MSC, 2005)	k = −11→13
T_{min} = 0.987, T_{max} = 0.991	l = −26→16
13910 measured reflections	

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
$R[F^2 > 2\sigma(F^2)]$ = 0.032	$w = 1/[\sigma^2(F_o^2) + (0.0475P)^2 + 0.1518P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.079	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.06	$\Delta\rho_{max}$ = 0.20 e $Å^{-3}$
2581 reflections	$\Delta\rho_{min}$ = −0.15 e $Å^{-3}$
251 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.032 (3)
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 $F^2 > \sigma(F^2)$ 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	0.07380 (13)	0.28900 (13)	0.73971 (6)	0.0287 (3)
O2	0.23820 (12)	0.17843 (12)	0.82576 (5)	0.0228 (3)
O3	0.38552 (14)	0.79457 (13)	0.92594 (6)	0.0329 (3)
O4	0.34335 (15)	0.69713 (14)	1.02429 (6)	0.0362 (3)
O5	0.96166 (13)	0.15373 (12)	0.87738 (6)	0.0226 (3)
H5	1.036 (2)	0.195 (2)	0.8592 (10)	0.034*
O6	1.04322 (12)	0.40766 (12)	0.88872 (6)	0.0241 (3)
C1	0.44649 (17)	0.48348 (17)	0.79244 (7)	0.0196 (3)
C2	0.35798 (18)	0.53926 (18)	0.74441 (8)	0.0230 (3)
H2	0.3827	0.6219	0.7246	0.028*
C3	0.23339 (18)	0.47622 (18)	0.72471 (8)	0.0247 (4)
H3	0.1747	0.5159	0.6917	0.030*
C4	0.19554 (17)	0.35649 (18)	0.75310 (8)	0.0226 (3)
C5	0.28519 (17)	0.29699 (17)	0.80056 (7)	0.0196 (3)
C6	0.40879 (17)	0.35955 (17)	0.81937 (7)	0.0192 (3)
H6	0.4693	0.3180	0.8511	0.023*
C7	−0.0319 (2)	0.3594 (2)	0.70329 (11)	0.0412 (5)
H7A	−0.0003	0.3730	0.6569	0.062*
H7B	−0.0485	0.4458	0.7246	0.062*
H7C	−0.1196	0.3079	0.7033	0.062*
C8	0.32263 (19)	0.11735 (19)	0.87673 (9)	0.0276 (4)
H8A	0.3305	0.1774	0.9153	0.041*
H8B	0.4168	0.0988	0.8588	0.041*
H8C	0.2784	0.0340	0.8910	0.041*
C9	0.57710 (16)	0.55340 (17)	0.81719 (7)	0.0209 (3)
H9A	0.6165	0.6068	0.7799	0.025*
H9B	0.6482	0.4855	0.8294	0.025*
C10	0.55425 (17)	0.64553 (16)	0.87818 (8)	0.0213 (3)
H10	0.6479	0.6827	0.8916	0.026*
C11	0.4557 (2)	0.76166 (18)	0.86314 (9)	0.0287 (4)
H11A	0.5100	0.8389	0.8464	0.034*
H11B	0.3856	0.7361	0.8286	0.034*
C12	0.39834 (18)	0.69247 (18)	0.96988 (8)	0.0257 (4)
C13	0.48662 (16)	0.58224 (16)	0.94058 (8)	0.0192 (3)
H13	0.4229	0.5086	0.9259	0.023*
C14	0.58852 (17)	0.52865 (17)	0.99399 (7)	0.0211 (3)
H14A	0.6435	0.6035	1.0129	0.025*
H14B	0.5334	0.4884	1.0310	0.025*
C15	0.68864 (17)	0.42650 (16)	0.96613 (8)	0.0194 (3)
C16	0.65324 (16)	0.29296 (17)	0.96147 (7)	0.0205 (3)
H16	0.5651	0.2633	0.9785	0.025*
C17	0.74541 (16)	0.20166 (17)	0.93208 (7)	0.0206 (3)

H17	0.7201	0.1105	0.9295	0.025*
C18	0.87370 (16)	0.24419 (16)	0.90675 (7)	0.0188 (3)
C19	0.91196 (16)	0.37751 (17)	0.91323 (7)	0.0187 (3)
C20	0.82073 (16)	0.46753 (17)	0.94260 (7)	0.0192 (3)
H20	0.8479	0.5580	0.9469	0.023*
C21	1.08409 (19)	0.54337 (18)	0.89079 (10)	0.0329 (4)
H21A	1.0905	0.5726	0.9376	0.049*
H21B	1.0139	0.5973	0.8671	0.049*
H21C	1.1761	0.5538	0.8691	0.049*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0263 (6)	0.0277 (7)	0.0322 (6)	−0.0037 (6)	−0.0070 (5)	0.0021 (5)
O2	0.0269 (6)	0.0178 (6)	0.0237 (5)	0.0014 (5)	0.0016 (5)	0.0025 (4)
O3	0.0430 (7)	0.0206 (6)	0.0353 (7)	0.0115 (6)	0.0054 (6)	0.0006 (5)
O4	0.0416 (7)	0.0322 (8)	0.0349 (7)	0.0107 (7)	0.0139 (6)	−0.0030 (6)
O5	0.0210 (5)	0.0180 (6)	0.0288 (6)	0.0004 (5)	0.0004 (5)	−0.0031 (5)
O6	0.0187 (5)	0.0194 (6)	0.0342 (6)	−0.0017 (5)	0.0050 (5)	−0.0041 (5)
C1	0.0205 (7)	0.0212 (8)	0.0171 (7)	0.0035 (7)	0.0033 (6)	0.0004 (6)
C2	0.0258 (8)	0.0209 (8)	0.0222 (8)	0.0017 (7)	0.0033 (6)	0.0036 (6)
C3	0.0247 (8)	0.0270 (9)	0.0222 (8)	0.0030 (7)	−0.0030 (6)	0.0041 (7)
C4	0.0225 (7)	0.0241 (9)	0.0214 (7)	0.0008 (7)	−0.0002 (6)	−0.0028 (6)
C5	0.0250 (8)	0.0159 (7)	0.0179 (7)	0.0034 (7)	0.0053 (6)	0.0007 (6)
C6	0.0218 (7)	0.0200 (8)	0.0158 (7)	0.0060 (7)	0.0023 (6)	−0.0002 (6)
C7	0.0310 (10)	0.0340 (11)	0.0584 (12)	−0.0034 (10)	−0.0192 (9)	0.0041 (10)
C8	0.0271 (8)	0.0259 (9)	0.0297 (9)	0.0047 (8)	0.0052 (7)	0.0108 (7)
C9	0.0193 (7)	0.0229 (8)	0.0206 (7)	0.0009 (7)	0.0030 (6)	0.0030 (6)
C10	0.0223 (7)	0.0177 (8)	0.0237 (7)	−0.0003 (7)	0.0015 (6)	0.0014 (6)
C11	0.0358 (9)	0.0193 (8)	0.0308 (9)	0.0049 (8)	0.0032 (7)	0.0029 (7)
C12	0.0250 (8)	0.0215 (8)	0.0307 (8)	0.0035 (7)	0.0022 (7)	−0.0025 (7)
C13	0.0187 (7)	0.0162 (8)	0.0227 (8)	0.0006 (6)	0.0017 (6)	−0.0015 (6)
C14	0.0213 (7)	0.0222 (8)	0.0198 (7)	0.0007 (7)	0.0028 (6)	0.0000 (6)
C15	0.0208 (7)	0.0223 (8)	0.0149 (7)	0.0024 (7)	−0.0018 (6)	0.0008 (6)
C16	0.0192 (7)	0.0220 (8)	0.0204 (7)	−0.0012 (7)	0.0001 (6)	0.0027 (6)
C17	0.0218 (7)	0.0182 (8)	0.0218 (7)	−0.0020 (7)	−0.0035 (6)	0.0019 (6)
C18	0.0193 (7)	0.0182 (8)	0.0190 (7)	0.0037 (6)	−0.0036 (6)	−0.0017 (6)
C19	0.0163 (7)	0.0217 (8)	0.0183 (7)	−0.0010 (6)	−0.0018 (6)	0.0009 (6)
C20	0.0204 (7)	0.0186 (8)	0.0188 (7)	−0.0003 (7)	−0.0023 (6)	−0.0009 (6)
C21	0.0260 (9)	0.0208 (9)	0.0519 (11)	−0.0064 (8)	0.0114 (8)	−0.0055 (8)

Geometric parameters (Å, °)

O1—C4	1.366 (2)	C9—C10	1.543 (2)
O1—C7	1.426 (2)	C9—H9A	0.9900
O2—C5	1.369 (2)	C9—H9B	0.9900
O2—C8	1.432 (2)	C10—C11	1.526 (2)
O3—C12	1.355 (2)	C10—C13	1.537 (2)
O3—C11	1.455 (2)	C10—H10	1.0000

O4—C12	1.203 (2)	C11—H11A	0.9900
O5—C18	1.3665 (19)	C11—H11B	0.9900
O5—H5	0.90 (2)	C12—C13	1.507 (2)
O6—C19	1.3712 (19)	C13—C14	1.535 (2)
O6—C21	1.421 (2)	C13—H13	1.0000
C1—C2	1.391 (2)	C14—C15	1.506 (2)
C1—C6	1.404 (2)	C14—H14A	0.9900
C1—C9	1.508 (2)	C14—H14B	0.9900
C2—C3	1.398 (2)	C15—C16	1.389 (2)
C2—H2	0.9500	C15—C20	1.400 (2)
C3—C4	1.379 (2)	C16—C17	1.397 (2)
C3—H3	0.9500	C16—H16	0.9500
C4—C5	1.405 (2)	C17—C18	1.385 (2)
C5—C6	1.383 (2)	C17—H17	0.9500
C6—H6	0.9500	C18—C19	1.396 (2)
C7—H7A	0.9800	C19—C20	1.383 (2)
C7—H7B	0.9800	C20—H20	0.9500
C7—H7C	0.9800	C21—H21A	0.9800
C8—H8A	0.9800	C21—H21B	0.9800
C8—H8B	0.9800	C21—H21C	0.9800
C8—H8C	0.9800		
C4—O1—C7	116.50 (15)	C9—C10—H10	108.1
C5—O2—C8	116.88 (13)	O3—C11—C10	106.62 (13)
C12—O3—C11	109.96 (13)	O3—C11—H11A	110.4
C18—O5—H5	109.9 (15)	C10—C11—H11A	110.4
C19—O6—C21	116.75 (13)	O3—C11—H11B	110.4
C2—C1—C6	117.88 (16)	C10—C11—H11B	110.4
C2—C1—C9	122.16 (15)	H11A—C11—H11B	108.6
C6—C1—C9	119.94 (14)	O4—C12—O3	120.85 (17)
C1—C2—C3	121.34 (16)	O4—C12—C13	128.17 (17)
C1—C2—H2	119.3	O3—C12—C13	110.98 (13)
C3—C2—H2	119.3	C12—C13—C14	109.88 (13)
C4—C3—C2	120.12 (15)	C12—C13—C10	103.87 (13)
C4—C3—H3	119.9	C14—C13—C10	116.31 (13)
C2—C3—H3	119.9	C12—C13—H13	108.8
O1—C4—C3	125.08 (15)	C14—C13—H13	108.8
O1—C4—C5	115.51 (16)	C10—C13—H13	108.8
C3—C4—C5	119.40 (16)	C15—C14—C13	112.45 (12)
O2—C5—C6	125.01 (14)	C15—C14—H14A	109.1
O2—C5—C4	114.90 (15)	C13—C14—H14A	109.1
C6—C5—C4	120.07 (15)	C15—C14—H14B	109.1
C5—C6—C1	121.14 (15)	C13—C14—H14B	109.1
C5—C6—H6	119.4	H14A—C14—H14B	107.8
C1—C6—H6	119.4	C16—C15—C20	118.66 (15)
O1—C7—H7A	109.5	C16—C15—C14	122.23 (15)
O1—C7—H7B	109.5	C20—C15—C14	119.10 (15)
H7A—C7—H7B	109.5	C15—C16—C17	120.90 (15)
O1—C7—H7C	109.5	C15—C16—H16	119.6
H7A—C7—H7C	109.5	C17—C16—H16	119.6

H7B—C7—H7C	109.5	C18—C17—C16	119.94 (15)
O2—C8—H8A	109.5	C18—C17—H17	120.0
O2—C8—H8B	109.5	C16—C17—H17	120.0
H8A—C8—H8B	109.5	O5—C18—C17	119.10 (15)
O2—C8—H8C	109.5	O5—C18—C19	121.42 (15)
H8A—C8—H8C	109.5	C17—C18—C19	119.46 (15)
H8B—C8—H8C	109.5	O6—C19—C20	125.01 (15)
C1—C9—C10	114.99 (13)	O6—C19—C18	114.57 (14)
C1—C9—H9A	108.5	C20—C19—C18	120.42 (15)
C10—C9—H9A	108.5	C19—C20—C15	120.55 (15)
C1—C9—H9B	108.5	C19—C20—H20	119.7
C10—C9—H9B	108.5	C15—C20—H20	119.7
H9A—C9—H9B	107.5	O6—C21—H21A	109.5
C11—C10—C13	102.73 (13)	O6—C21—H21B	109.5
C11—C10—C9	113.07 (13)	H21A—C21—H21B	109.5
C13—C10—C9	116.48 (13)	O6—C21—H21C	109.5
C11—C10—H10	108.1	H21A—C21—H21C	109.5
C13—C10—H10	108.1	H21B—C21—H21C	109.5
C6—C1—C2—C3	1.7 (2)	O3—C12—C13—C14	137.62 (14)
C9—C1—C2—C3	−176.52 (14)	O4—C12—C13—C10	−167.32 (18)
C1—C2—C3—C4	0.2 (2)	O3—C12—C13—C10	12.54 (18)
C7—O1—C4—C3	−11.9 (2)	C11—C10—C13—C12	−21.56 (16)
C7—O1—C4—C5	167.03 (16)	C9—C10—C13—C12	−145.71 (14)
C2—C3—C4—O1	177.18 (15)	C11—C10—C13—C14	−142.41 (14)
C2—C3—C4—C5	−1.7 (2)	C9—C10—C13—C14	93.44 (17)
C8—O2—C5—C6	1.7 (2)	C12—C13—C14—C15	−174.92 (14)
C8—O2—C5—C4	−176.99 (13)	C10—C13—C14—C15	−57.32 (19)
O1—C4—C5—O2	1.0 (2)	C13—C14—C15—C16	−85.45 (19)
C3—C4—C5—O2	179.99 (14)	C13—C14—C15—C20	93.00 (17)
O1—C4—C5—C6	−177.79 (13)	C20—C15—C16—C17	−1.9 (2)
C3—C4—C5—C6	1.2 (2)	C14—C15—C16—C17	176.52 (14)
O2—C5—C6—C1	−177.86 (14)	C15—C16—C17—C18	−0.4 (2)
C4—C5—C6—C1	0.8 (2)	C16—C17—C18—O5	−179.14 (13)
C2—C1—C6—C5	−2.2 (2)	C16—C17—C18—C19	2.5 (2)
C9—C1—C6—C5	176.05 (13)	C21—O6—C19—C20	−3.5 (2)
C2—C1—C9—C10	89.17 (18)	C21—O6—C19—C18	176.67 (15)
C6—C1—C9—C10	−89.02 (18)	O5—C18—C19—O6	−0.7 (2)
C1—C9—C10—C11	−63.25 (19)	C17—C18—C19—O6	177.63 (13)
C1—C9—C10—C13	55.42 (19)	O5—C18—C19—C20	179.43 (14)
C12—O3—C11—C10	−17.30 (19)	C17—C18—C19—C20	−2.2 (2)
C13—C10—C11—O3	23.87 (17)	O6—C19—C20—C15	−179.96 (14)
C9—C10—C11—O3	150.24 (14)	C18—C19—C20—C15	−0.1 (2)
C11—O3—C12—O4	−177.32 (17)	C16—C15—C20—C19	2.2 (2)
C11—O3—C12—C13	2.8 (2)	C14—C15—C20—C19	−176.31 (14)
O4—C12—C13—C14	−42.2 (2)		

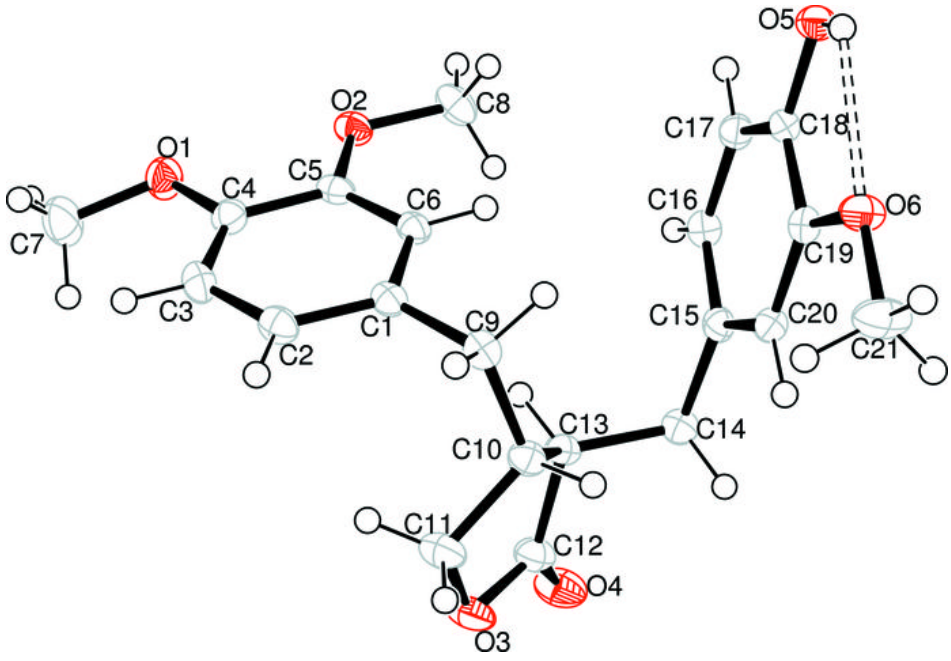
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

O5—H5···O2^{i}	0.90 (2)	2.04 (2)	2.8280 (17)	146 (2)
O5—H5···O6	0.90 (2)	2.22 (2)	2.6799 (18)	111.7 (17)
O5—H5···O1^{i}	0.90 (2)	2.58 (2)	3.2406 (18)	130.8 (16)
C3—H3···O5^{ii}	0.95	2.34	3.278 (2)	168
C14—H14A···O4^{iii}	0.99	2.86	3.687 (2)	142
C14—H14B···O5^{iv}	0.99	2.42	3.373 (2)	162
C20—H20···O4^{iii}	0.95	2.53	3.446 (2)	162

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

Fig. 1


O5
O2
C8
C17
C18
O1
C5
C4
C16
O6
C6
C7
C19
C3
C15
C20
C1
C9
C21
C2
C13
C14
C10
C11
C12
O4
O3