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(2*R*,4*S*,5*S*)-5-Methoxy-4-methyl-3-oxohept-6-en-2-yl benzoate

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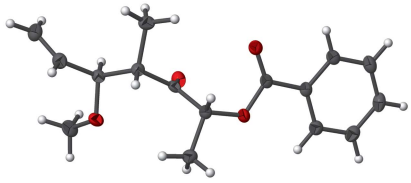
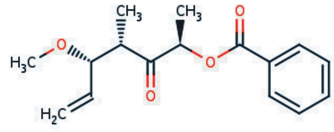
The title compound, $C_{16}H_{20}O_4$, was synthesized in the course of the total synthesis of fusaequisin A in order to verify and confirm the configurations of the stereogenic centers and to exclude the possibility of epimerization during the methylation process. The crystal structure of the title compound at 100 K has orthorhombic ($P2_12_12_1$) symmetry. The absolute configuration was determined by anomalous dispersion and agrees with the configuration of the allylic alcohol used in the synthesis.

3D view



Chemical scheme



Structure description

The title compound, $C_{16}H_{20}O_4$ (Fig. 1), was obtained during the synthesis of the Western fragment of fusaequisin A. Background to fusaequisin A is given by Shiono *et al.* (2013). The asymmetric synthesis of the Western fragment is based on Paterson's *anti* aldol chemistry (Paterson *et al.*, 1994; Paterson, 1998). In the course of the total synthesis of curvicollide C (Che *et al.*, 2004) the precursor of the title compound (**I**) was prepared (von Kiedrowski *et al.*, 2017) and provided potential for further investigations regarding the total synthesis of fusaequisin A. The methylation process is shown in Fig. 2.

The title compound crystallizes in the orthorhombic space group $P2_12_12_1$ with four molecules in the unit cell with H1*A* and H3*A* almost in plane (H1*A*—C1···C3—H3*A* pseudo torsion angle = −1°) and H2*A* and H3*A* in an antiperiplanar arrangement (H2*A*—C2—C3—H3*A* = 179°), which minimizes 1,3-allylic strain. Furthermore, the C8 methyl group and the O1 atom of the ether group are also in an antiperiplanar arrangement with a C8—C4—C3—O1 torsion angle of 177.32 (10)°. The ester moiety shows the most stable and expected *s*–*cis*-conformation. In the crystal, a weak C—H···O interaction arising from the aromatic C—H grouping *para* to the side chain links the molecules into *C*(10) chains propagating in the [010] direction (Table 1).

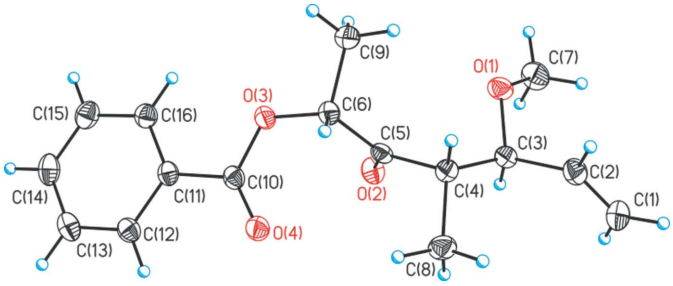


Figure 1
The molecular structure of **I** showing displacement ellipsoids at the 50% probability level

Synthesis and crystallization

The reaction (Fig. 3) was carried out under an argon atmosphere. To an ice-cooled solution of the allylic alcohol ($C_{15}H_{18}O_4$, 262.31 g mol^{-1}, 300 mg, 1.10 mmol, 1 equiv.) in CH_2Cl_2 were successively added dried (0.1 mbar, 250°C, 2 h) 3 Å molecular sieves (200 mg), 1,8-bis(dimethylamino)-naphthalene (proton sponge®, $C_{14}H_{18}N_2$, 214.31 g mol^{-1}, 943 mg, 4.40 mmol, 4 equiv.) and trimethyloxonium tetrafluoroborate (Me_3OBF_4, $C_3H_9BF_4O$, 147.91 g mol^{-1}, 651 mg, 4.40 mmol, 4 equiv.). The opaque, orange solution was warmed to room temperature. The reaction mixture was stirred at room temperature for 4 h and was then diluted by the addition of aqueous phosphate pH 7 buffer. The phases were separated and the aqueous layer was extracted three times with CH_2Cl_2. The combined organic layers were dried ($MgSO_4$) and all volatiles were removed under reduced pressure. The light yellow residue was purified by flash chromatography (cyclohexane-ethyl acetate, 20:1 to 10:1) to afford the title methyl ether (**I**) ($C_{16}H_{20}O_4$, 276.33 g mol^{-1}, 238 mg, 0.86 mmol, 78%) as a white solid. Colourless crystals of **I** suitable for X-ray crystallographic analysis were obtained under air by slow evaporation from the mixed solvents of diethyl ether and *n*-pentane. R_f = 0.56 (cyclohexane–ethyl acetate, 5:1); m.p. = 80–83°C; $[\alpha]_D^{20}$ = −8.3° (*c* = 0.5 g ml^{-1} in $CHCl_3$) ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.06 (*d*, *J* = 7.1 Hz, 3H, 3-CH_3), 1.55 (*d*, *J* = 7.0 Hz, 3H, 1-CH_3), 2.93 (*dq*, *J* = 9.7, 7.1 Hz, 1H, 3-CH), 3.15 (*s*, 3H, 4-OCH_3), 3.70 (*dd*, *J* = 10.1, 9.3 Hz, 1H, 4-CH), 5.24–5.35 (*m*, 2H, 6-CH_2), 5.41 (*q*, *J* = 7.0 Hz, 1H, 1-CH), 5.56 (*ddd*, *J* = 17.1, 10.1, 8.5 Hz, 1H, 5-CH), 7.43–7.48 (*m*, 2H, aryl-CH), 7.55–7.60 (*m*, 1H, aryl-CH), 8.05–8.12 (*m*, 2H, aryl-CH); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 14.1 (3-CH_3), 15.3 (1-CH_3), 47.0 (3-

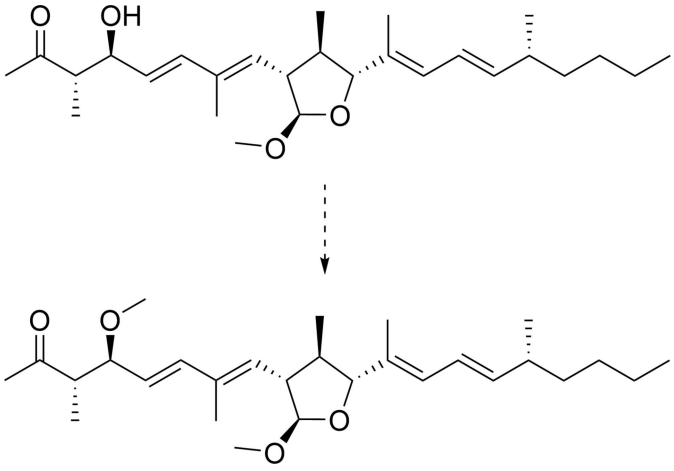


Figure 2
Methylation of *O*-desmethylfusaequisin A.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14*A*···O2^{i}	0.95	2.54	3.2838 (18)	135

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{20}O_4$
M_r	276.32
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	100
a, *b*, *c* (Å)	8.1297 (4), 11.8232 (6), 15.7213 (9)
V (Å^3)	1511.12 (14)
Z	4
Radiation type	Cu *K*α
μ (mm^{-1})	0.71
Crystal size (mm)	0.12 × 0.10 × 0.06
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*;Bruker, 2016)
T_{min}, T_{max}	0.700, 0.754
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28627, 3078, 3054
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.023, 0.060, 1.07
No. of reflections	3078
No. of parameters	184
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.18, −0.12
Absolute structure	Flack *x* determined using 1293 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.03 (2)

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *XP* (Sheldrick, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

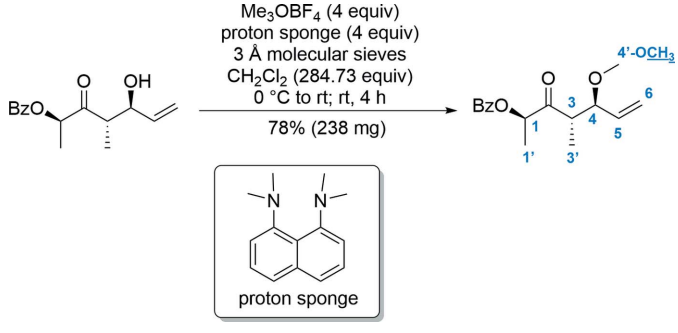


Figure 3
Reaction conditions for the methylation of the allylic alcohol.

CH), 56.6 (4-OCH_3), 75.5 (1-CH), 85.4 (4-CH), 120.2 (6-CH_2), 128.5 (aryl-CH), 129.8 (aryl-CH), 129.9 (aryl-CH), 133.3 (aryl-CH), 136.0 (5-CH), 166.0 (aryl-C), 210.1 (2-C); **IR** ν = 3075 (*w*), 2985 (*w*), 2935 (*w*), 2825 (*w*), 1720 (*s*), 1065 (*w*), 1450 (*m*), 1420 (*w*), 1375 (*m*), 1315 (*m*), 1265 (*s*), 1205 (*w*), 1175 (*w*), 1115 (*s*), 1090 (*s*), 1070 (*m*), 1025 (*m*), 1010 (*m*), 965 (*m*), 935 (*m*), 715 (*s*), 685 (*w*) cm^{-1}; **HRMS (ESI)**: *m*/*z* $[M + H]^+$ calculated for $C_{16}H_{21}O_4$: 277.1434; found: 277.1342.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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full crystallographic data

IUCrData (2021). **6**, x210951 [https://doi.org/10.1107/S2414314621009512]

(2*R*,4*S*,5*S*)-5-Methoxy-4-methyl-3-oxohept-6-en-2-yl benzoate

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Crystal data

$C_{16}H_{20}O_4$
M_r = 276.32
Orthorhombic, $P2_12_12_1$
a = 8.1297 (4) Å
b = 11.8232 (6) Å
c = 15.7213 (9) Å
V = 1511.12 (14) Å^3
Z = 4
F(000) = 592
D_x = 1.215 Mg m^{-3}
Melting point = 353–356 K
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9807 reflections
θ = 6.1–74.6°
μ = 0.71 mm^{-1}
T = 100 K
Block, colourless
0.12 × 0.10 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS;Bruker, 2016)
T_{min} = 0.700, T_{max} = 0.754
28627 measured reflections
3078 independent reflections
3054 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 74.5°, θ_{min} = 4.7°
h = −10→10
k = −14→14
l = −18→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.060
S = 1.07
3078 reflections
184 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0308P)^2 + 0.2127P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}
Absolute structure: Flack x determined using 1293 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.03 (2)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.09507 (18)	0.29265 (12)	0.39623 (10)	0.0306 (3)
H1A	0.080921	0.309404	0.337584	0.037*
H1B	0.010147	0.255322	0.426807	0.037*
O1	0.52090 (11)	0.31350 (8)	0.40027 (6)	0.0257 (2)
C2	0.23199 (17)	0.32109 (12)	0.43502 (9)	0.0260 (3)
H2A	0.241816	0.302998	0.493680	0.031*
O2	0.57315 (12)	0.55222 (8)	0.31396 (6)	0.0257 (2)
C3	0.37402 (15)	0.38013 (10)	0.39331 (8)	0.0210 (3)
H3A	0.348192	0.392678	0.331840	0.025*
O3	0.79670 (11)	0.67523 (7)	0.40634 (6)	0.02254 (19)
C4	0.41493 (15)	0.49330 (10)	0.43492 (8)	0.0200 (2)
H4A	0.442788	0.480340	0.496105	0.024*
O4	0.58296 (11)	0.79534 (7)	0.39300 (6)	0.0255 (2)
C5	0.56184 (15)	0.54690 (10)	0.39052 (8)	0.0195 (2)
C6	0.69017 (16)	0.59668 (11)	0.45003 (8)	0.0214 (3)
H6A	0.633436	0.636762	0.497741	0.026*
C7	0.5209 (2)	0.22018 (12)	0.34321 (10)	0.0346 (3)
H7A	0.624899	0.178862	0.348492	0.052*
H7B	0.508591	0.247754	0.284770	0.052*
H7C	0.429206	0.169617	0.357046	0.052*
C8	0.27180 (16)	0.57771 (12)	0.42921 (10)	0.0279 (3)
H8A	0.180721	0.551481	0.464968	0.042*
H8B	0.234674	0.583387	0.370058	0.042*
H8C	0.308649	0.652131	0.448962	0.042*
C9	0.80093 (17)	0.50522 (12)	0.48637 (10)	0.0298 (3)
H9A	0.733683	0.448423	0.515567	0.045*
H9B	0.878182	0.539103	0.526875	0.045*
H9C	0.862385	0.469110	0.440132	0.045*
C10	0.72720 (16)	0.77408 (10)	0.38331 (7)	0.0204 (3)
C11	0.85150 (16)	0.85390 (10)	0.34781 (8)	0.0206 (3)
C12	0.79937 (18)	0.96224 (11)	0.32518 (8)	0.0237 (3)
H12A	0.686828	0.982661	0.330513	0.028*
C13	0.91308 (19)	1.04000 (11)	0.29482 (9)	0.0286 (3)
H13A	0.878073	1.114116	0.280093	0.034*
C14	1.07716 (19)	1.01054 (12)	0.28578 (9)	0.0303 (3)
H14A	1.153904	1.064064	0.264420	0.036*
C15	1.12937 (17)	0.90223 (13)	0.30810 (9)	0.0294 (3)
H15A	1.241701	0.881748	0.301761	0.035*
C16	1.01703 (17)	0.82427 (11)	0.33962 (8)	0.0243 (3)
H16A	1.052798	0.750788	0.355613	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0290 (7)	0.0303 (7)	0.0325 (7)	−0.0065 (6)	0.0030 (6)	0.0020 (6)

O1	0.0265 (4)	0.0206 (4)	0.0298 (5)	0.0050 (4)	−0.0010 (4)	−0.0022 (4)
C2	0.0284 (7)	0.0248 (6)	0.0249 (6)	−0.0012 (5)	0.0023 (5)	0.0032 (5)
O2	0.0317 (5)	0.0244 (4)	0.0211 (4)	−0.0027 (4)	0.0034 (4)	−0.0001 (3)
C3	0.0220 (6)	0.0199 (6)	0.0210 (6)	0.0009 (5)	0.0000 (5)	0.0011 (5)
O3	0.0210 (4)	0.0178 (4)	0.0289 (5)	−0.0008 (4)	0.0021 (4)	0.0021 (4)
C4	0.0197 (5)	0.0207 (6)	0.0197 (5)	0.0004 (5)	0.0012 (5)	−0.0017 (5)
O4	0.0226 (4)	0.0211 (4)	0.0326 (5)	0.0007 (4)	0.0033 (4)	−0.0017 (4)
C5	0.0215 (6)	0.0146 (5)	0.0224 (6)	0.0040 (5)	0.0012 (5)	0.0001 (5)
C6	0.0210 (6)	0.0199 (6)	0.0234 (6)	−0.0018 (5)	0.0013 (5)	0.0028 (5)
C7	0.0377 (8)	0.0236 (6)	0.0426 (8)	0.0051 (6)	0.0039 (7)	−0.0090 (6)
C8	0.0234 (6)	0.0264 (7)	0.0339 (7)	0.0053 (5)	0.0006 (6)	−0.0059 (5)
C9	0.0233 (6)	0.0279 (7)	0.0382 (7)	−0.0005 (6)	−0.0036 (6)	0.0095 (6)
C10	0.0244 (6)	0.0174 (5)	0.0196 (6)	−0.0006 (5)	−0.0008 (5)	−0.0030 (5)
C11	0.0245 (6)	0.0192 (6)	0.0180 (6)	−0.0020 (5)	0.0002 (5)	−0.0034 (5)
C12	0.0277 (7)	0.0209 (6)	0.0226 (6)	0.0005 (5)	0.0004 (5)	−0.0015 (5)
C13	0.0389 (7)	0.0214 (6)	0.0256 (6)	−0.0034 (6)	0.0022 (6)	0.0009 (5)
C14	0.0354 (7)	0.0296 (7)	0.0260 (6)	−0.0119 (6)	0.0064 (6)	−0.0015 (5)
C15	0.0252 (7)	0.0340 (7)	0.0291 (7)	−0.0038 (6)	0.0038 (5)	−0.0049 (6)
C16	0.0257 (6)	0.0236 (6)	0.0235 (6)	−0.0003 (5)	0.0003 (5)	−0.0026 (5)

Geometric parameters (Å, º)

C1—C2	1.313 (2)	C7—H7B	0.9800
C1—H1A	0.9500	C7—H7C	0.9800
C1—H1B	0.9500	C8—H8A	0.9800
O1—C7	1.4220 (17)	C8—H8B	0.9800
O1—C3	1.4347 (15)	C8—H8C	0.9800
C2—C3	1.5001 (18)	C9—H9A	0.9800
C2—H2A	0.9500	C9—H9B	0.9800
O2—C5	1.2087 (16)	C9—H9C	0.9800
C3—C4	1.5261 (17)	C10—C11	1.4911 (18)
C3—H3A	1.0000	C11—C12	1.3953 (18)
O3—C10	1.3477 (15)	C11—C16	1.3965 (19)
O3—C6	1.4438 (15)	C12—C13	1.3883 (19)
C4—C5	1.5215 (17)	C12—H12A	0.9500
C4—C8	1.5357 (17)	C13—C14	1.386 (2)
C4—H4A	1.0000	C13—H13A	0.9500
O4—C10	1.2089 (16)	C14—C15	1.394 (2)
C5—C6	1.5199 (17)	C14—H14A	0.9500
C6—C9	1.5188 (18)	C15—C16	1.389 (2)
C6—H6A	1.0000	C15—H15A	0.9500
C7—H7A	0.9800	C16—H16A	0.9500
C2—C1—H1A	120.0	H7B—C7—H7C	109.5
C2—C1—H1B	120.0	C4—C8—H8A	109.5
H1A—C1—H1B	120.0	C4—C8—H8B	109.5
C7—O1—C3	112.20 (11)	H8A—C8—H8B	109.5
C1—C2—C3	124.65 (12)	C4—C8—H8C	109.5

C1—C2—H2A	117.7	H8A—C8—H8C	109.5
C3—C2—H2A	117.7	H8B—C8—H8C	109.5
O1—C3—C2	110.60 (10)	C6—C9—H9A	109.5
O1—C3—C4	105.50 (10)	C6—C9—H9B	109.5
C2—C3—C4	112.85 (10)	H9A—C9—H9B	109.5
O1—C3—H3A	109.3	C6—C9—H9C	109.5
C2—C3—H3A	109.3	H9A—C9—H9C	109.5
C4—C3—H3A	109.3	H9B—C9—H9C	109.5
C10—O3—C6	115.73 (10)	O4—C10—O3	123.58 (12)
C5—C4—C3	109.85 (10)	O4—C10—C11	124.96 (12)
C5—C4—C8	107.29 (10)	O3—C10—C11	111.42 (11)
C3—C4—C8	112.31 (10)	C12—C11—C16	119.97 (12)
C5—C4—H4A	109.1	C12—C11—C10	118.07 (12)
C3—C4—H4A	109.1	C16—C11—C10	121.92 (12)
C8—C4—H4A	109.1	C13—C12—C11	119.56 (13)
O2—C5—C6	122.72 (12)	C13—C12—H12A	120.2
O2—C5—C4	122.56 (12)	C11—C12—H12A	120.2
C6—C5—C4	114.69 (10)	C14—C13—C12	120.64 (13)
O3—C6—C9	106.34 (10)	C14—C13—H13A	119.7
O3—C6—C5	111.60 (10)	C12—C13—H13A	119.7
C9—C6—C5	111.27 (11)	C13—C14—C15	119.88 (13)
O3—C6—H6A	109.2	C13—C14—H14A	120.1
C9—C6—H6A	109.2	C15—C14—H14A	120.1
C5—C6—H6A	109.2	C16—C15—C14	119.95 (13)
O1—C7—H7A	109.5	C16—C15—H15A	120.0
O1—C7—H7B	109.5	C14—C15—H15A	120.0
H7A—C7—H7B	109.5	C15—C16—C11	120.00 (13)
O1—C7—H7C	109.5	C15—C16—H16A	120.0
H7A—C7—H7C	109.5	C11—C16—H16A	120.0

C7—O1—C3—C2	75.42 (14)	O2—C5—C6—C9	−102.56 (14)
C7—O1—C3—C4	−162.25 (11)	C4—C5—C6—C9	79.43 (13)
C1—C2—C3—O1	−121.33 (15)	C6—O3—C10—O4	−4.44 (17)
C1—C2—C3—C4	120.75 (15)	C6—O3—C10—C11	173.50 (10)
O1—C3—C4—C5	58.00 (12)	O4—C10—C11—C12	1.17 (19)
C2—C3—C4—C5	178.86 (10)	O3—C10—C11—C12	−176.74 (11)
O1—C3—C4—C8	177.32 (10)	O4—C10—C11—C16	178.96 (13)
C2—C3—C4—C8	−61.81 (14)	O3—C10—C11—C16	1.06 (16)
C3—C4—C5—O2	46.33 (16)	C16—C11—C12—C13	−0.16 (19)
C8—C4—C5—O2	−76.02 (15)	C10—C11—C12—C13	177.67 (11)
C3—C4—C5—C6	−135.66 (10)	C11—C12—C13—C14	0.8 (2)
C8—C4—C5—C6	101.99 (12)	C12—C13—C14—C15	−0.6 (2)
C10—O3—C6—C9	−167.80 (11)	C13—C14—C15—C16	−0.2 (2)
C10—O3—C6—C5	70.68 (13)	C14—C15—C16—C11	0.9 (2)
O2—C5—C6—O3	16.05 (17)	C12—C11—C16—C15	−0.70 (19)
C4—C5—C6—O3	−161.96 (10)	C10—C11—C16—C15	−178.45 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14*A*···O2^{i}	0.95	2.54	3.2838 (18)	135

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