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(1*R*,2*R*,3*S*,4*S*)-2-[(2*R*,3*S*)-2,3-Dimethyloxiran-2-yl]-3,4-bis(4-methoxybenzyloxy)cyclohexanol

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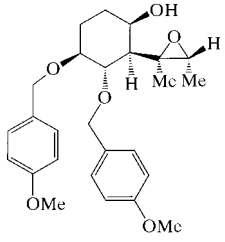
The relative configuration was determined for the title compound, $C_{26}H_{34}O_6$, which was prepared in a synthetic study on immunosuppressant FR65814. There is an intramolecular hydrogen bond between the hydroxy and epoxy groups.

Comment

The total synthesis of novel immunosuppressant FR65814 was



(I)

reported (Amano *et al.*, 1998, 1999). The title compound, (I), was prepared in a synthetic study on FR65814.

Experimental

The title compound was synthesized from D-glucose (Amano *et al.*, 1999). The stereochemistries at C-3 and C-4 (atom labels C3 and C4, respectively) came from those at C-2 and C-3 of D-glucose, respectively.

Crystal data

$C_{26}H_{34}O_6$
M_r = 442.55
Orthorhombic, $P2_12_12_1$
a = 18.060 (3) Å
b = 23.477 (3) Å
c = 5.736 (2) Å
V = 2431 (1) Å^3
Z = 4
D_x = 1.209 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10–15°
μ = 0.085 mm^{-1}
T = 296 K
Prism, colourless
0.6 × 0.4 × 0.4 mm

Data collection

Rigaku AFC-5*S* diffractometer
θ–2θ scans
2493 measured reflections
2493 independent reflections
1281 reflections with $I > 2\sigma(I)$
θ_{max} = 25°
$h = 0 \rightarrow 21$
$k = 0 \rightarrow 28$
$l = 0 \rightarrow 7$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R(F)$ = 0.073
$wR(F^2)$ = 0.221
S = 1.92
2493 reflections
292 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + \{0.05(F_o^2 + 2F_c^2)/3\}^2]$
$(\Delta/\sigma)_{max}$ = 0.010
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: see text, no Friedel pairs

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.429 (10)	O3—C3	1.457 (8)
O2—C7	1.45 (1)	O5—C4	1.424 (8)
O2—C8	1.411 (10)	C7—C8	1.49 (1)
C7—O2—C8	62.7 (5)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.96	1.73	2.673 (9)	166

The positional parameters of all the H atoms were calculated geometrically and fixed with U(H) = 1.2U_{eq}(parent atom). The absolute structure was assigned based on the known absolute configurations around the C3 and C4 atoms, which came from D-glucose.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

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