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(2*S*,3*R*,4*S*,5*R*,6*S*)-6-Benzyloxymethyl-4-(methoxymethyloxy)-9-oxo-8-oxa-1-azabicyclo[4.3.0]nonane-2,3,5-triyl triacetate

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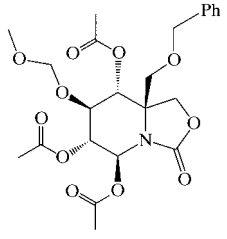
The relative configuration of the title compound, $C_{23}H_{29}NO_{11}$, prepared in a synthetic study on the natural product *sphingofungin E*, has been determined. The six-membered ring adopts a chair form and the five substituents are all axial.

Comment

The title compound, (I), was synthesized in a synthetic study on *sphingofungin E* (Oishi *et al.*, 2000). The stereochemistries



(I)

at C-3, C-4 and C-5 (atom labels C2, C3 and C4, respectively) came from those at C-2, C-3 and C-4 of D-glucose, respectively.

Experimental

The title compound, (I), was synthesized from D-glucose. The crystals were grown from a toluene solution.

Crystal data

$C_{23}H_{29}NO_{11}$
M_r = 495.48
Tetragonal, $P4_3$
a = 14.381 (2) Å
c = 12.265 (2) Å
V = 2536.4 (7) Å^3
Z = 4
D_x = 1.297 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10–15°
μ = 0.104 mm^{-1}
T = 296 K
Prism, colourless
0.5 × 0.5 × 0.5 mm

Data collection

Rigaku AFC-5*S* diffractometer
θ–2θ scans
2844 measured reflections
2621 independent reflections
1656 reflections with $I > 2\sigma(I)$
R_{int} = 0.010
θ_{max} = 26°
$h = 0 \rightarrow 18$
$k = 0 \rightarrow 18$
$l = 0 \rightarrow 15$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R(F)$ = 0.047
$wR(F^2)$ = 0.116
S = 1.19
2621 reflections
324 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + \{0.05(F_o^2 + 2F_c^2)/3\}^2]$
$(\Delta/\sigma)_{max}$ = 0.026
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Absolute structure: see text, no Friedel pairs

Table 1
Selected geometric parameters (Å).

O1—C6	1.436 (5)	O7—C3	1.422 (5)
O1—C7	1.352 (5)	O9—C4	1.445 (5)
O2—C7	1.197 (6)	N1—C1	1.429 (5)
O3—C1	1.441 (5)	N1—C5	1.459 (5)
O5—C2	1.452 (5)	N1—C7	1.354 (5)

There are two possible conformations of the methoxymethyloxy group. The site-occupation factors of O7—C12—O8—C13 and O7—C14—O8—C15 were assumed to be 65 and 35%, respectively. The C14 and C15 atoms were refined isotropically. 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 C2, 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*.

References

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Molecular Structure Corporation (1993). *MSC/AFC Diffractometer Control Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Molecular Structure Corporation (1999). *TEXSAN*. Version 1.10. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Oishi, T., Ando, K., Inomiya, K. & Chida, N. (2000). In preparation.