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## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.030  
 $wR$  factor = 0.085  
Data-to-parameter ratio = 6.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

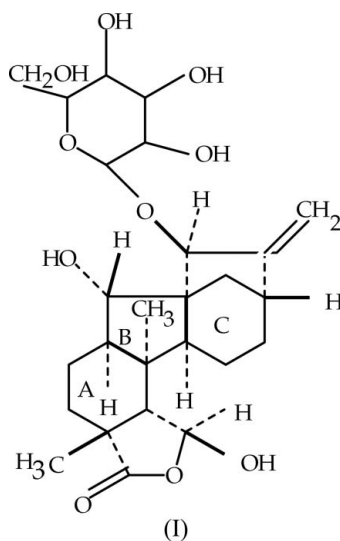
## Farnesiaside, a new diterpene glycoside

In the title compound,  $\text{C}_{26}\text{H}_{38}\text{O}_{10}$ , the acafarnane skeleton consists of three *cis*-fused rings, of which the five-membered ring is in an envelope conformation and the two six-membered rings adopt twist-boat and chair conformations. The lactone ring is in an envelope conformation. The *D*-glucose, in the  $\beta$  position with respect to the acafarnane skeleton, adopts a chair conformation. The molecular structure and the crystal packing are stabilized by  $\text{O}-\text{H}\cdots\text{O}$  interactions including a bifurcated hydrogen bond.

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## Comment

The title compound, a novel diterpene glycoside, has been isolated from the seeds of *Acacia farnesiana* Willd. *A. farnesiana*, a thorny bush or small tree, which is native to tropical America and cosmopolitan in the tropics. It has become naturalized in almost all parts of India and is used as folk remedy for different ailments (Chadha, 1985). The isolation and characterization of the compound have been performed and it has been designated as farnesiaside, possessing a new carbon skeleton to which the name acafarnane has been recommended (Sahu *et al.*, 1997). The present X-ray structural analysis has been undertaken to confirm the results obtained from spectroscopic studies.



The molecule (Fig. 1) consists of a kaurene-derived acafarnane skeleton to which a lactone ring is fused and *D*-glucose is attached at C15 in the  $\beta$  position. The acafarnane skeleton consists of three *cis*-fused rings, *A* (atoms C1–C5, C10), *B* (C1, C7–C10) and *C* (C8/C9/C11–C14). Ring *A* is in twist-boat conformation. The five-membered ring *B* adopts an

envelope conformation with C8 at the flap. The six-membered ring *C* is in a chair conformation. The methyl group at C10 and the hydroxyl group at C7 are in axial positions. The lactone ring *D* is in an envelope conformation with C5 at the flap. The methyl group C19 is in an axial position. The  $\beta$ -D-glucose ring is in a chair conformation. The ring puckering parameters for rings *A*, *B*, *C*, *D* (C4–C6, O1, C18) and *E* (C21, O6, C22–C25) (Cremer & Pople, 1975) are given in Table 3.

The OH group (O4), attached to the acafarnane skeleton is hydrogen-bonded to two O atoms (O5 and O10) of the D-glucose unit, forming a bifurcated hydrogen bond. Atom O9 of the D-glucose unit is involved in an intermolecular hydrogen bond with atom O7. Atom O10 also forms an intermolecular hydrogen bond with O8. The O atom (O2) of the hydroxyl group of the lactone ring is involved in an intermolecular hydrogen bond with O9. The hydrogen-bond details are given in Table 2.

### Experimental

The air-dried powdered seeds of *A. farnesiana* (1 kg) were successively extracted with light petrol(60–80°), CHCl<sub>3</sub> and MeOH in a soxhlet extractor. The concentrated MeOH extract was partitioned between *n*-BuOH and H<sub>2</sub>O. The *n*-BuOH extract was washed with H<sub>2</sub>O and evaporated under reduced pressure to give a dark-brown powder (5.8 g). This solid was taken up in MeOH (150 ml) and filtered. The concentrated filtrate was kept in the refrigerator for 48 h; crystals separated out, and were identified as D-glucose by PC and specific rotation. The mother liquor was dried to give a dark-brown mass (4.6 g) which was chromatographed over a column of silica gel (60 g). Farnesiaside was eluted with a CHCl<sub>3</sub>–MeOH mixture (9:1). Crystals were obtained by slow evaporation of a MeOH solution at room temperature.

#### Crystal data

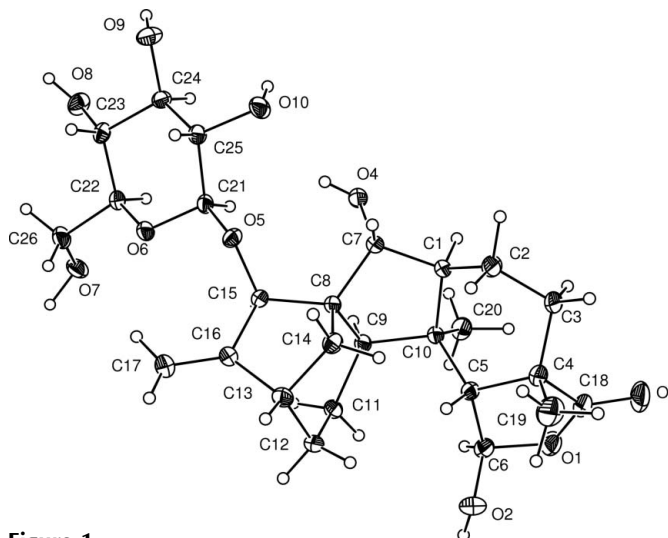
C<sub>26</sub>H<sub>38</sub>O<sub>10</sub>  
*M<sub>r</sub>* = 510.56  
 Monoclinic, *P*2<sub>1</sub>  
*a* = 11.691 (2) Å  
*b* = 9.336 (3) Å  
*c* = 12.370 (2) Å  
 $\beta$  = 114.82 (3)°  
*V* = 1225.4 (6) Å<sup>3</sup>  
*Z* = 2  
*D<sub>x</sub>* = 1.384 Mg m<sup>-3</sup>  
 Cu *K* $\alpha$  radiation  
 $\mu$  = 0.88 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Prism, pale yellow  
 0.21 × 0.16 × 0.13 mm

#### Data collection

Siemens AED diffractometer  
 $\theta$ – $2\theta$  scans  
 Absorption correction: none  
 2585 measured reflections  
 2511 independent reflections  
 2446 reflections with *I* > 2 $\sigma$ (*I*)  
*R<sub>int</sub>* = 0.038  
 $\theta_{\max}$  = 70.1°  
 1 standard reflection  
 every 100 reflections  
 intensity decay: none

#### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.030  
*wR*(*F*<sup>2</sup>) = 0.085  
*S* = 1.04  
 2511 reflections  
 372 parameters  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0669P)^2 + 0.1111P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta\sigma)_{\max} = 0.004$   
 $\Delta\rho_{\max} = 0.21 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.17 \text{ e \AA}^{-3}$   
 Extinction correction: *SHELXL97*  
 Extinction coefficient: 0.0058 (7)



**Figure 1**  
 Structure of the compound showing 30% probability displacement ellipsoids and the atom numbering.

**Table 1**

Selected geometric parameters (Å, °).

C6–O2	1.379 (3)	C18–O3	1.214 (3)
C6–O1	1.470 (3)	C18–O1	1.335 (3)
C16–C17	1.321 (3)		
C17–C16–C13	126.4 (2)	O3–C18–C4	125.9 (2)
C17–C16–C15	125.24 (19)	C18–O1–C6	110.53 (16)
O3–C18–O1	121.9 (2)		
C19–C4–C5–C6	–92.7 (2)	C5–C4–C18–O3	167.3 (3)
C4–C5–C6–O2	94.6 (2)	C19–C4–C18–O1	104.2 (2)
C4–C5–C10–C20	81.0 (2)	O3–C18–O1–C6	177.3 (3)
C2–C1–C10–C20	–112.4 (2)	O2–C6–O1–C18	–102.4 (2)

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
O4–H4O...O5	0.82	2.43	2.952 (2)	122
O4–H4O...O10	0.82	2.08	2.866 (3)	161
O2–H2O...O9 <sup>i</sup>	0.82	2.09	2.868 (3)	157
O8–H8O...O3 <sup>ii</sup>	0.82	1.85	2.664 (3)	172
O9–H9O...O7 <sup>iii</sup>	0.82	2.02	2.815 (2)	164
O10–H10O...O8 <sup>iii</sup>	0.82	2.03	2.832 (2)	168
O7–H7O...O4 <sup>iv</sup>	0.82	2.02	2.835 (2)	170

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

**Table 3**

Ring-puckering parameters (Å, °) for five rings.

Ring	<i>q</i> <sub>2</sub>	<i>q</i> <sub>3</sub>	<i>Q</i> <sub>T</sub>	$\theta$
<i>A</i>	0.672 (2)	–0.133 (2)	0.685 (2)	101.2 (2)
<i>B</i>	0.372 (2)			
<i>C</i>	0.260 (2)	–0.570 (2)	0.627 (2)	155.5 (2)
<i>D</i>	0.242 (2)			
<i>E</i>	0.056 (2)	–0.572 (2)	0.574 (2)	174.4 (2)

All H atoms were refined using a riding model with C–H = 0.98 Å,  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for methine, C–H = 0.97 Å,  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for methylene, C–H = 0.93 Å,  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for aromatic, C–H = 0.96 Å,  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl and C–H = 0.93 Å,  $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$  for ethylene H atoms. Hydroxyl H atoms were refined with O–H = 0.82 Å,  $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{O})$ . The hydroxyl and methyl groups were allowed to rotate but not to tip. In the absence of significant scattering effects, the Flack (1983) parameter was indeterminate. Hence the Friedal equivalents were merged, and the absolute configuration was assigned by reference to the known chirality of related compounds.

Data collection: *AED Software* (Belletti *et al.*, 1993); cell refinement: *AED Software*; data reduction: *AED Software*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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