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## Key indicators

Single-crystal X-ray study  
 $T = 295\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.011\text{ \AA}$   
H-atom completeness 99%  
Disorder in solvent or counterion  
 $R$  factor = 0.068  
 $wR$  factor = 0.189  
Data-to-parameter ratio = 8.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.A taxane diterpenoid from the heartwood of *Taxus wallichiana*In the title compound, 5-acetyl-2-deacetoxydecinnamoyltaxinine 0.29-hydrate,  $\text{C}_{30}\text{H}_{42}\text{O}_{10} \cdot 0.29\text{H}_2\text{O}$ , the eight-membered ring adopts a boat-like conformation. The molecule as a whole adopts a cage-type folded conformation.Received 16 October 2001  
Accepted 16 January 2002  
Online 25 January 2002CIMAP Communication No.  
2001-53Jb.

## Comment

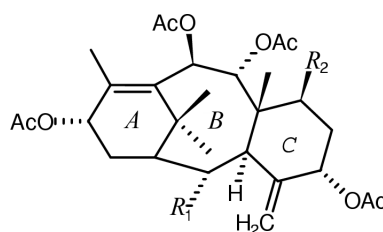
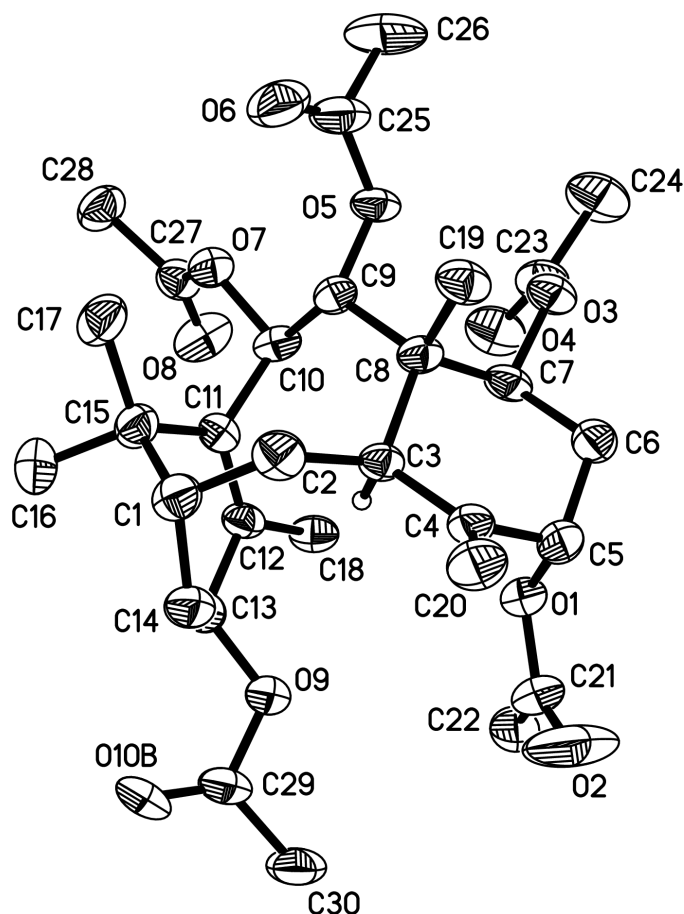
Investigations on the taxoid constituents of different parts of *Taxus wallichiana* led to isolation of the title compound, (I)·0.29H<sub>2</sub>O. Taxoid (I), which was isolated from the heartwood and roots of *T. wallichiana*, was found to be isomeric with taxa-4-(2)*O*,11-diene-2 $\alpha$ ,5 $\alpha$ ,9 $\alpha$ ,10 $\beta$ ,13 $\alpha$ -pentaol pentaacetate, (II), isolated from the heartwood of *T. Baccata* (Della Casa de Marcano & Halsall, 1969). Considerable attention has been given to this type of diterpenoid molecule whose archetype is paclitaxel (Taxol<sup>TM</sup>), a promising cancer chemotherapeutic agent (Appendino, 1995). Although numerous X-ray investigations have been performed on this and related molecules, there is much heated debate about the active conformation of this anticancer drug (Mastro Paolo *et al.*, 1995). This prompted us to undertake the present X-ray study on the title compound.(I)  $R_1 = \text{H}$ ,  $R_2 = \text{OAc}$ (II)  $R_1 = \text{OAc}$ ,  $R_2 = \text{H}$ 

Fig. 1 shows the conformation and molecular structure of (I)·0.29H<sub>2</sub>O with the atomic numbering scheme. The torsion angles of the terpenoid core of the molecule are listed in Table 1. The molecule contains a fused three-ring system A/B/C. The B/C junction is *trans*-fused due to the *trans*-axial dispositions of C19 at C8 and H3 at C3. Least-squares planes calculations indicate that the eight-membered B ring is folded to form a boat-like conformation [the deviations of atoms C9, C2, C15 and C1 are 0.601 (7), 1.300 (8), 1.406 (8) and 1.346 (7) Å, respectively, from the mean plane through atoms C3, C8, C10 and C11]. The six-membered ring C adopts a chair conformation, while ring A adopts a distorted envelope conformation [the deviation of atom C15 is −0.833 (6) Å from the mean plane through atoms C1, C11, C12, C13 and C14]. The mole-



**Figure 1**  
Displacement ellipsoid plot (30% probability) showing the atom labelling. Only one H atom (H3) is shown to indicate its relative disposition at the B/C ring junction. Also, only the major component (60%) of the disordered atom O10 is shown.

cule as a whole adopts a folded cage-type conformation. Three short intramolecular H $\cdots$ H contacts (H2A $\cdots$ H20B 1.87 Å, H9 $\cdots$ H17A 1.80 Å and H13 $\cdots$ H16C 1.83 Å) are observed in the structure. The presence of these short contacts may be due to the sterically strained nature of the molecule.

## Experimental

The title compound was isolated from the methanol extracts of the heartwood of *T. wallichiana* following reported protocols (Chattopadhyay *et al.*, 1999). Diffraction-quality crystals were grown by slow evaporation of a methanolic solution at room temperature.

### Crystal data

C<sub>30</sub>H<sub>42</sub>O<sub>10</sub>·0.29H<sub>2</sub>O  
*M<sub>r</sub>* = 567.86  
 Orthorhombic, *P*2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>  
*a* = 11.252 (2) Å  
*b* = 16.003 (3) Å  
*c* = 16.801 (2) Å  
*V* = 3025.3 (9) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 1.247 Mg m<sup>-3</sup>

Mo *K*α radiation  
 Cell parameters from 64 reflections  
 $\theta$  = 2.4–12.8°  
 $\mu$  = 0.09 mm<sup>-1</sup>  
*T* = 295 (2) K  
 Block, colourless  
 0.36 × 0.32 × 0.25 mm

### Data collection

Bruker P4 diffractometer  
 $\theta$ -2 $\theta$  scans  
 Absorption correction: none  
 4177 measured reflections  
 3321 independent reflections  
 1699 reflections with *I* > 2 $\sigma$ (*I*)  
*R*<sub>int</sub> = 0.027  
 $\theta$ <sub>max</sub> = 26.0°

*h* = -13 → 1  
*k* = -1 → 19  
*l* = -1 → 20  
 3 standard reflections  
 every 97 reflections  
 frequency: 60 min  
 intensity decay: none

### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.068  
*wR*(*F*<sup>2</sup>) = 0.189  
*S* = 1.03  
 3321 reflections  
 383 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 3.3578P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.24 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.24 \text{ e } \text{Å}^{-3}$

**Table 1**

Selected torsion angles (°).

C14–C1–C2–C3	52.5 (8)	C7–C8–C9–C10	63.0 (7)
C15–C1–C2–C3	-73.7 (8)	C3–C8–C9–C10	-55.1 (8)
C1–C2–C3–C4	-122.3 (6)	C8–C9–C10–C11	62.2 (8)
C1–C2–C3–C8	109.1 (7)	C9–C10–C11–C12	-113.3 (7)
C2–C3–C4–C5	172.3 (6)	C9–C10–C11–C15	58.2 (8)
C8–C3–C4–C5	-57.7 (8)	C10–C11–C12–C13	163.3 (6)
C3–C4–C5–C6	54.0 (8)	C15–C11–C12–C13	-8.3 (10)
C4–C5–C6–C7	-54.0 (9)	C11–C12–C13–C14	-33.8 (10)
C5–C6–C7–C8	60.0 (9)	C12–C13–C14–C1	23.5 (10)
C6–C7–C8–C9	179.2 (5)	C15–C1–C14–C13	24.4 (10)
C6–C7–C8–C3	-58.1 (7)	C2–C1–C14–C13	-103.8 (8)
C4–C3–C8–C9	178.8 (6)	C12–C11–C15–C1	56.1 (8)
C2–C3–C8–C9	-51.0 (8)	C10–C11–C15–C1	-115.6 (7)
C4–C3–C8–C7	55.8 (7)	C14–C1–C15–C11	-60.9 (7)
C2–C3–C8–C7	-174.0 (5)	C2–C1–C15–C11	66.7 (7)

All H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms for the final cycles of refinement. The absolute structure could not be established (Flack, 1983) because of the weak anomalous signal. Friedel reflections were merged for the final cycles of refinement. A solvent water molecule was observed at a hydrogen-bonding distance of 2.71 (3) Å from atom O4 of the taxoid molecule. The solvent oxygen (O11) behaved badly on refinement (disordered with lower occupancy). Atom O11 was refined isotropically. H atoms of the water molecule could not be located from the difference Fourier map.

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL-NT* (Bruker, 1997); program(s) used to refine structure: *SHELXTL-NT*; molecular graphics: *SHELXTL-NT*; software used to prepare material for publication: *SHELXTL-NT*.

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