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Furanoeudesmane-B, a new eudesmane sesquiterpenoid from *Myoporum bontioides*

Qiguang Wang,[a]* Chunling Ma[a] and Jianjun Zhai[b]

[a]Lanzhou University, Lanzhou, Gansu 730000, People's Republic of China, and [b]Instrumental Analysis and Research Center, Lanzhou University, Lanzhou, Gansu 730000, People's Republic of China
Correspondence e-mail: wangqg@lzu.edu.cn

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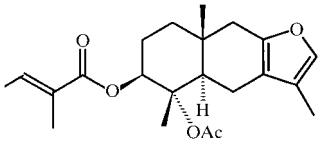
Myoporum bontioides is a folk medicinal plant from the northwest of China and is known as a superficies-syndrome drug. The EtOH extract from the dried root of *Myoporum bontioides* was chromatographed to give furanoeudesmane-B, a new eudesmane sesquiterpenoid. The structure of furanoeudesmane-B (3β-angloyloxy-4α-acetoxy-5αH-furanoeudesmane), $C_{22}H_{30}O_5$, has not been determined by X-ray crystallography before.

Comment

In the course of a search for bioactive drugs, *Myoporum bontioides*, which is widespread in the northwest of China, was selected as it has efficiency as an antipyretic and detoxicate, and is used for relieving uneasiness and fever in folk medicine. A study with somewhat larger amounts of the plant material and careful chromatography have allowed the isolation of 3β-angloyloxy-4α-acetoxy-5αH-furanoeudesmane, named furanoeudesmane-B. The title compound, (I), was a new eudesmane



(I)

sesquiterpenoid. Several similar eudesmane derivatives (Bohlmann & Zdero, 1977) and quite a few eremophilane sesquiterpenoids (Bohlmann *et al.*, 1978; Bohlmann & Zdero, 1979), which have the same elemental composition as the title compound, have been reported previously.

The skeleton of furanoeudesmane consists of two six-membered rings and a furan ring connected together (labelled *A*–*C* left-to-right in the Scheme). Ring *A* (C1–C5 and C10) takes a chair conformation, with C4 0.653 (3) Å above and C1 0.609 (4) Å below the plane; ring *B* (C5–C10) takes a half-chair conformation as a result of the neighbouring furan ring, with C10 0.662 (3) Å above. Furan ring *C* (C7, C8, C11, C12 and O1) is essentially planar, including the C13 methyl group. The dihedral angle between the planar parts of rings *A* and *B* is 32.4 (2)°, and 34.0 (2)° between the planar segments of *A* and *C*; the planar segments of *B* and *C* are almost coplanar, the dihedral angle being only 4.6 (2)°.

Experimental

The EtOH extract of *Myoporum bontioides* was chromatographed on a silica-gel column using the stepwise solvent gradient method (EtOH/petroleum ether). The title compound was obtained from the 12% EtOH/petroleum ether fraction (0.02% dry wt) and crystallized from EtOH yielding colourless crystals (m.p. 474–475 K). Its molecular formula was determined as $C_{22}H_{30}O_5$ from the mass spectrum and elemental analysis. The experimental sample was recrystallized from ethyl alchol/acetone.

Crystal data

$C_{22}H_{30}O_5$	Mo $K\alpha$ radiation
M_r = 374.46	Cell parameters from 20 reflections
Orthorhombic, $P2_12_12_1$	θ = 8.02–15.47°
a = 8.854 (1) Å	μ = 0.091 mm^{-1}
b = 12.122 (1) Å	T = 293 (2) K
c = 17.708 (2) Å	Block, colourless
V = 1900.6 (3) Å^3	0.4 × 0.3 × 0.2 mm
Z = 4	
D_x = 1.309 Mg m^{-3}	

Data collection

Enraf–Nonius CAD-4 diffractometer	θ_{max} = 28.72°
ω–2θ scans	$h = -10 \rightarrow 10$
4692 measured reflections	$k = 0 \rightarrow 14$
2348 independent reflections	$l = 0 \rightarrow 23$
2348 reflections with $F^2 > 0$	3 standard reflections
R_{int} = 0.048	frequency: 60 min
	intensity decay: 0.1%

Refinement

Refinement on F^2	H-atom parameters not refined
$R[F^2 > 2\sigma(F^2)]$ = 0.040	$w = 1/[\sigma^2(F_o^2) + (0.1253P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.039	$(\Delta/\sigma)_{max}$ = 0.011
S = 1.421	$\Delta\rho_{max}$ = 0.34 e Å^{-3}
2347 reflections	$\Delta\rho_{min}$ = −0.23 e Å^{-3}
244 parameters	

Data collection and cell refinement: *CAD*-4 *Users Manual* (Enraf–Nonius, 1985); data reduction: *Xtal*3.4 *ADDREF SORTRF* (Hall *et al.*, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *Xtal*3.4 *CRYLSQ*; molecular graphics: *Xtal*3.4; software used to prepare material for publication: *Xtal*3.4 *BONDLA CIFIO*.

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