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(10*S*,13*R*,14*R*)-17-(2-Hydroxy-1,5-dimethylhex-4-enyl)-4,4,10,13,14-pentamethyl-2,3,4,5,6,7,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-ol

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.007 Å
R factor = 0.051
wR factor = 0.139
Data-to-parameter ratio = 9.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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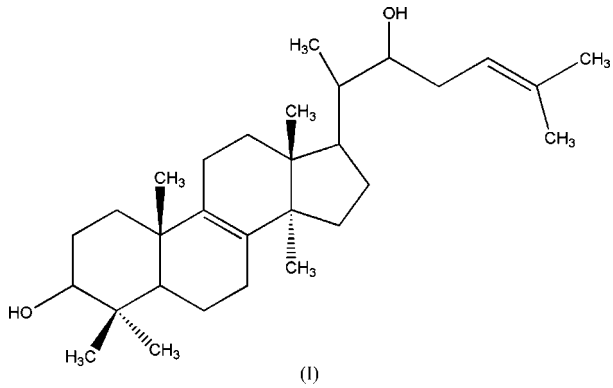
The title compound, $C_{30}H_{50}O_2$, was isolated from the wood-rotting fungus *Inonotus obliquus*. It is a lanostane-type triterpene. There are one cyclohexane ring, two cyclohexene rings and one cyclopentane ring in the molecule.

Comment

Inonotus obliquus (Fr.) Pilat (Hymenochaetaceae), a parasitic basidiomycete fungus usually found growing on living trunks of mature birch trees, is predominantly distributed in the far east of Russia, northeastern China and other adjacent countries at latitudes of 45–50 N. This fungus has been used to treat various diseases in Russia, Poland and most of the Baltic countries for more than 100 years. Over this time, *Inonotus obliquus* has demonstrated a peculiar efficacy in treating patients suffering from breast cancer, hepatoma, gastrointestinal cancer and other cancers of the digestive organs without incurring any unacceptable toxicity (Huang, 2002). The title compound, (I), has been extracted from *Inonotus obliquus* (Rufina & Urszula, 1958). A significant anticancer effect of the title compound from the fungus is observed on Walker 256 carcinosarcoma and MCF-7 human mammary adenocarcinoma (Shin, 2001).



(I)

The molecule of (I) contains one cyclohexane ring, two cyclohexene rings and one cyclopentane ring (Fig. 1). Ring *A* (atoms C1/C2/C5–C8) adopts a chair conformation, and rings *B* (atoms C1/C8/C10–C13), *C* (atoms C10/C11/C14/C15/C16/C18) and *D* (atoms C16/C18/C20/C21/C22) adopt envelope conformations.

The crystal packing is stabilized by intermolecular hydrogen bonding (Fig. 2).

Experimental

Powdered *Inonotus obliquus* (3 kg) was extracted five times with 80% ethanol at room temperature for 24 h per extraction. The ethanol

extracts were combined and concentrated under reduced pressure. The concentrated extracts were successively separated on macroporous resin (ADS-17), EtOH–H_2O (70:1 *v*/*v*) and a silica-gel column (CC, Wako gel C-200), CH_3Cl–MeOH (60:1 *v*/*v*), affording the title compound. Single crystals suitable for X-ray diffraction were obtained by the slow evaporation of an ethanol solution of the title compound.

Crystal data

$C_{30}H_{50}O_2$
M_r = 442.70
Orthorhombic, $P2_12_12_1$
a = 7.4504 (11) Å
b = 12.746 (2) Å
c = 28.639 (6) Å
V = 2719.7 (9) Å^3
Z = 4
D_x = 1.081 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2191 reflections
θ = 2.8–26.3°
μ = 0.07 mm^{-1}
T = 294 (2) K
Plate, white
0.24 × 0.22 × 0.04 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.985, T_{max} = 0.997
13212 measured reflections
2759 independent reflections
1563 reflections with $I > 2\sigma(I)$
R_{int} = 0.088
θ_{max} = 25.0°
$h = -8 \rightarrow 8$
$k = -14 \rightarrow 15$
$l = -19 \rightarrow 34$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.139
S = 1.08
2759 reflections
300 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0365P)^2 + 1.7113P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0026 (5)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	2.01	2.825 (5)	175
O2—H2···O1^{ii}	0.82	2.22	2.775 (5)	125

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

All H atoms were placed in geometrically idealized positions (O—H = 0.82 Å and C—H = 0.96–0.98 Å) and allowed to ride on their parent atoms, with U_{iso}(H) values set at $1.5U_{eq}$(C) for the methyl H atoms and at $1.2U_{eq}$(C,O) for other H atoms. In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXL97*.

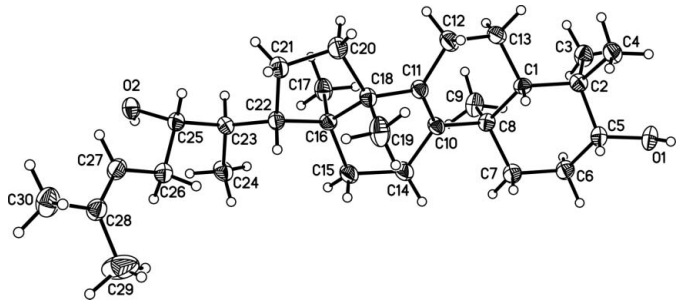


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

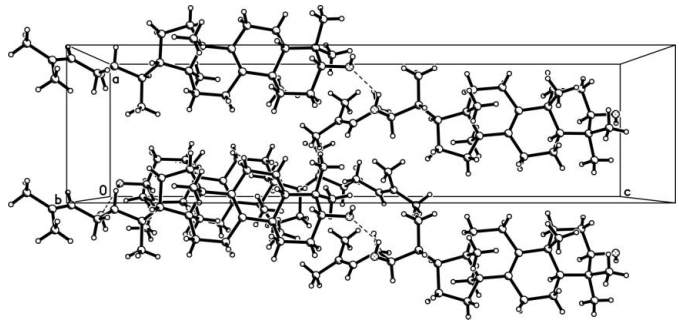


Figure 2
The molecular packing of (I). Dashed lines indicate hydrogen bonds.

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