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#### Key indicators

Single-crystal X-ray study  
 T = 85 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$   
 R factor = 0.046  
 wR factor = 0.121  
 Data-to-parameter ratio = 20.1

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

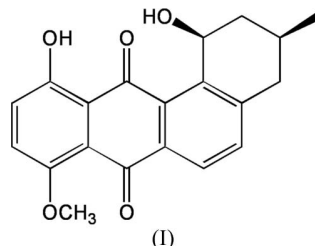
## rac-Hatomarubigin C

The title compound [systematic name: (1*RS*,3*RS*)-1,11-dihydroxy-8-methoxy-3-methyl-1,2,3,4-tetrahydrobenzo[*a*]-anthracene-7,11-dione],  $\text{C}_{20}\text{H}_{18}\text{O}_5$ , crystallizes with two molecules in the asymmetric unit. Each molecule exhibits a curvature of the anthraquinone ring system and possesses two intramolecular  $\text{C}=\text{O} \cdots \text{H}-\text{O}$  hydrogen bonds. Pairs of enantiomers form  $\pi$ -stacked dimers, with this interaction supported by intermolecular hydrogen bonds.

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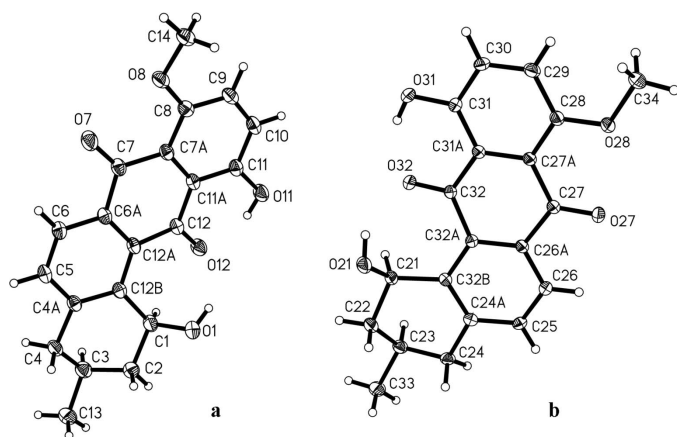
### Comment

Hatomarubigin C, (I), is an angucycline antibiotic which was isolated from the culture broth of *Streptomyces* sp. 2238-SVT4 (Hayakawa *et al.*, 1991). It has been found to potentiate the activity of the anticancer drug colchicine against colchicine-resistant cancer kB ( $\text{CH}^R$ ) cell lines *in vitro*. As part of an ongoing programme studying these compounds, we developed a synthesis of (I), albeit in racemic form (Caygill *et al.*, 1997). We report here the crystal structure of (I) (Fig. 1).



Two molecules of (I) are found in the asymmetric unit; in the arbitrary choice of asymmetric unit in this centrosymmetric structure, the two molecules are enantiomers. Small differences in the geometric parameters are observed between the two molecules. Fig. 1 clearly shows the benzo[*a*]-anthraquinone nucleus (ring system) of (I). Furthermore, the C1–OH and C3 methyl groups of the hydroaromatic *A* ring (atoms C1–C12*B* and C21–C32*B*) are *cis*-related. Both of these substituents possess a pseudo-equatorial orientation. Both molecules show a curvature of the anthraquinone ring system, with angles between the planes of the *B* (atoms C6*A*–C12*A* and C26*A*–C32*A*) and *D* (atoms C7*A*–C11*A* and C27*A*–C31*A*) rings of 8.03 (5) and 8.91 (4)°. The 11-OH (31-OH) group forms an intramolecular hydrogen bond to carbonyl atom O12 (O32). A second, weaker, hydrogen bond exists between the 1-OH (21-OH) group and carbonyl atom O12 (O32) (Fig. 2 and Table 1).

Consideration of the molecular packing shows pairs of enantiomers form  $\pi$ -stacked head-to-tail dimers (Fig. 2), with an angle between the anthraquinone planes of 15.9 (2)° and a closest C  $\cdots$  C distance of 3.336 (3) Å. The dimer is further



**Figure 1**

The structure of the two molecules of (I) (a and b) in the asymmetric unit, showing displacement ellipsoids at the 50% probability level.

stabilized by complementary intermolecular hydrogen bonds between the OH substituents (1-OH, 21-OH) on the A rings of each molecule (Table 1). These OH substituents are therefore bifurcating, being involved in both intra- and intermolecular hydrogen bonding. The dimers stack in columns parallel to the crystallographic *a* axis (Figs. 2 and 3), with a closest C...C distance between dimers of 3.295 (2) Å. Various weak intermolecular C—H...O=C hydrogen bonds between these stacks of dimers complete the stabilization of the packing.

## Experimental

The title compound was prepared as described by Caygill *et al.* (1997). Suitable single crystals were obtained as red rods from a mixture of dichloromethane, diethyl ether and hexanes (1:1:2).

### Crystal data

C<sub>20</sub>H<sub>18</sub>O<sub>5</sub>  
*M<sub>r</sub>* = 338.34  
 Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 14.273 (3) Å  
*b* = 17.066 (3) Å  
*c* = 12.958 (3) Å  
 $\beta$  = 95.25 (3)°  
*V* = 3143.2 (11) Å<sup>3</sup>

*Z* = 8  
*D<sub>x</sub>* = 1.430 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 $\mu$  = 0.10 mm<sup>-1</sup>  
*T* = 85 (2) K  
 Rod, red  
 0.49 × 0.12 × 0.12 mm

### Data collection

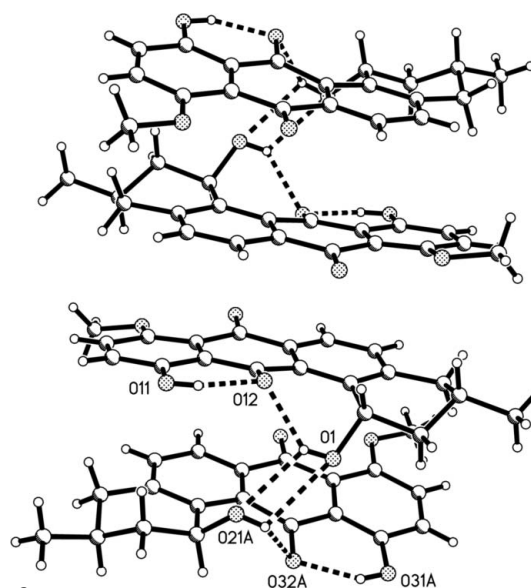
Bruker Kappa-APEXII area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (APEX2; Bruker, 2004)  
*T<sub>min</sub>* = 0.985, *T<sub>max</sub>* = 0.988

81294 measured reflections  
 9162 independent reflections  
 7375 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.032  
*R<sub>max</sub>* = 33.3°

### Refinement

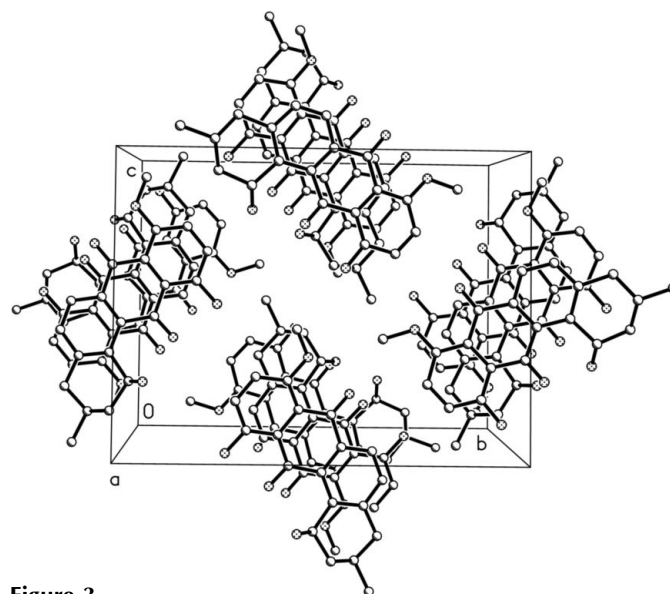
Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.046  
*wR*(*F*<sup>2</sup>) = 0.121  
*S* = 1.06  
 9162 reflections  
 455 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0498P)^2 + 1.8289P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.69 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.27 \text{ e } \text{Å}^{-3}$



**Figure 2**

Views of two of the  $\pi$ -stacked dimers, showing the intra- and intermolecular hydrogen bonds drawn as dashed lines. Atoms labelled with the suffix A are at the symmetry position  $(x - y + \frac{3}{2}, z - \frac{1}{2})$ .



**Figure 3**

A view of the molecular packing of (I). H atoms have been omitted for clarity.

**Table 1**

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>
O11—H11...O12	0.82	1.78	2.5050 (14)	146
O31—H31...O32	0.82	1.81	2.5207 (14)	145
O1—H1...O12	0.82	2.01	2.6574 (16)	135
O21—H21A...O32	0.82	2.01	2.6583 (13)	135
O1—H1...O21 <sup>i</sup>	0.82	2.35	2.8620 (15)	121
O21—H21A...O1 <sup>ii</sup>	0.82	2.45	2.8620 (15)	112

Symmetry codes: (i)  $x, -y + \frac{3}{2}, z - \frac{1}{2}$ ; (ii)  $x, -y + \frac{3}{2}, z + \frac{1}{2}$ .

All H atoms were refined using a riding model, with C—H = 0.93 Å and *U<sub>iso</sub>*(H) = 1.2*U<sub>eq</sub>*(C) for aromatic C atoms, C—H = 0.96 Å and

$U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for aliphatic C atoms, and  $\text{O}-\text{H} = 0.82 \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$  for OH groups.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *APEX2*; program(s) used to refine structure: *APEX2*; molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: *enCIFer* (Version 1.1; Allen *et al.*, 2004).

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