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#### Key indicators

Single-crystal X-ray study  
T = 273 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$   
R factor = 0.039  
wR factor = 0.105  
Data-to-parameter ratio = 8.9

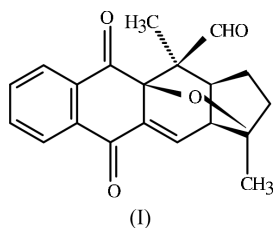
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## The natural naphthoquinone sterekunthal-B

The title structure, 15,18-dimethyl-5-dioxo-14-oxapentacyclo-[11.4.1.0<sup>2,15</sup>.0<sup>4,13</sup>.0<sup>6,11</sup>]octadeca-3,6,8,10-tetraene-18-carbaldehyde, C<sub>20</sub>H<sub>18</sub>O<sub>4</sub>, is a novel naphthoquinone, isolated from *Stereospermum personatum*. In the bicyclic system, all three six-membered rings adopt a boat conformation. Two intermolecular C=O...H—C interactions link the molecules into a chain.

#### Comment

*Stereospermum personatum* is a well known medicinal plant, frequently used in the Ayurvedic system of medicine. The plant belongs to the *Bignoniaceae* family which is known for its antimicrobial, antiprotozoal and anti-inflammatory properties (Binutu *et al.*, 1996). A recent report on antimalarial ingredients from *Stereospermum kunthianum* prompted us to systematically isolate the ingredients from *Stereospermum personatum*, a locally available plant. The natural naphthoquinone sterekunthal-B, (I), has previously been isolated from *Stereospermum kunthianum* (Onegi *et al.*, 2002) and its structure was established on the basis of spectroscopic and chemical evidence. Recently, it has also been isolated from *Stereospermum personatum* (Sampath Kumar *et al.*, 2003). This structure has been confirmed by our X-ray diffraction study, the results of which are presented here.



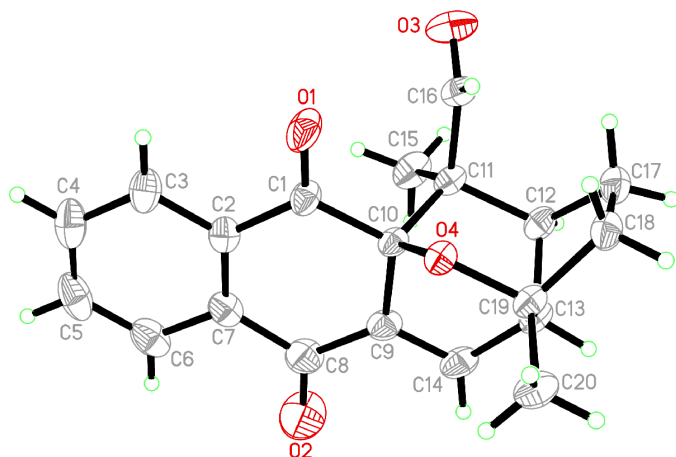
All bond lengths and angles are normal and are in good agreement with related structures reported in the literature (Joshi *et al.*, 1982). The title compound, (I), contains a naphthoquinone ring system and an aldehyde-substituted bicyclic system. Additionally, a five-membered ring shares the two C atoms of the bicyclic ring system. The naphthoquinone ring system is almost planar, with an average deviation from the least-squares plane through atoms C1–C10 of 0.027 (2) Å. Quinone atoms O1 and O2 are situated almost in this ring plane, with displacements of 0.094 (2) and 0.004 (3) Å, respectively.

The bicyclic system has, in principle, *D*<sub>3</sub> symmetry; however, the presence of substituents leads to deviations from the ideal geometry. This can be seen from the torsion angles (Table 1) and the puckering parameters (Cremer & Pople, 1975). In the

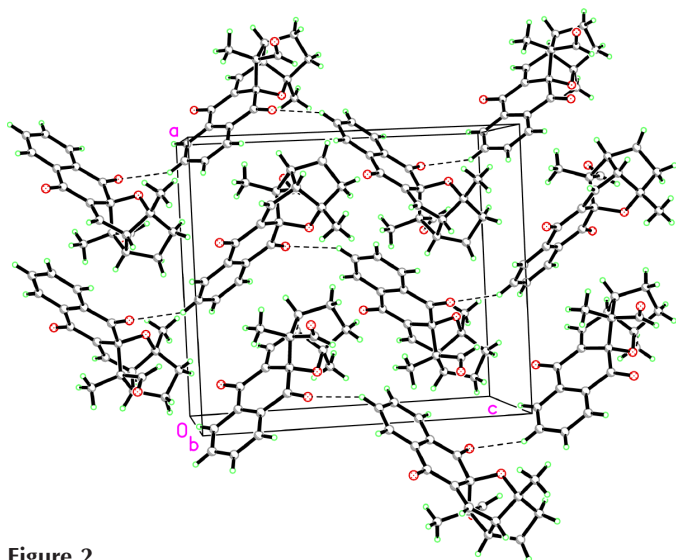
Received 18 January 2005

Accepted 24 January 2005

Online 29 January 2005



**Figure 1**  
A view of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.



**Figure 2**  
The wave-like packing of the molecules linked by C–H...O interactions (dashed lines), viewed down the *b* axis.

bicyclic fragment, all three six-membered rings adopt a boat conformation:  $q_2 = 0.780$  (2) Å,  $q_3 = 0.081$  (2) Å,  $\varphi = -66.2$  (2)°,  $\theta = 84.1$  (1)° and  $Q_t = 0.784$  (2) Å for the C9–C14 ring;  $q_2 = 0.932$  (2) Å,  $q_3 = -0.091$  (2) Å,  $\varphi = -61.9$  (1)°,  $\theta = 95.6$  (1)° and  $Q_t = 0.936$  (2) Å for the C10–C13/C19/O4 ring, and  $q_2 = 1.344$  (13) Å,  $q_3 = 0.038$  (2) Å,  $\varphi = -179.4$  (1)°,  $\theta = 88.4$  (1)° and  $Q_t = 1.345$  (13) Å for the C9/C10/C13/C14/C19/O4 ring.

The five-membered C12/C13/C17–C19 ring adopts an envelope conformation, as evidenced by the puckering parameters  $q_2 = 0.982$  (3) Å and  $\varphi_2 = 23.8$  (1)°, with atom C13 displaced by  $-0.767$  (2) Å from the mean plane of the rest of the atoms.

The C15 methyl group is in an axial orientation, while the C16=O aldehyde group is in an equatorial position with respect to the C9–C14 ring. Similarly, the C20 methyl group at ring junction C19 is in an equatorial orientation with respect to the five-membered ring.

Two intermolecular C=O...H–C interactions (Table 2) exist, involving atoms O1 (2.55 Å to H5) and O3 (2.47 Å to H13). Both these distances lie within the 2.7 Å range, generally employed for non-bonded H...O packing interactions (Steiner, 1997). These may be viewed as ‘weak hydrogen bonds’ with significant contribution to packing forces, based on the compiled data for a large number of C–H...O contacts (Steiner & Desiraju, 1998), rather than simple van der Waals attractions.

## Experimental

The title compound was isolated as pale-yellow solid by chromatographic methods from the petroleum ether extract of the stem bark of the plant *Stereospermum personatum* (Sampath Kumar *et al.*, 2003). Crystals suitable for X-ray analysis were obtained from methanol.

### Crystal data

$C_{20}H_{18}O_4$	Mo $K\alpha$ radiation
$M_r = 322.34$	Cell parameters from 6143 reflections
Orthorhombic, $Pna2_1$	$\theta = 2.7\text{--}27.9^\circ$
$a = 13.3078$ (19) Å	$\mu = 0.09$ mm <sup>-1</sup>
$b = 7.9299$ (11) Å	$T = 273$ (2) K
$c = 15.168$ (2) Å	Block, pale yellow
$V = 1600.7$ (4) Å <sup>3</sup>	$0.25 \times 0.13 \times 0.10$ mm
$Z = 4$	
$D_x = 1.338$ Mg m <sup>-3</sup>	

### Data collection

Bruker SMART APEX CCD area-detector diffractometer	1879 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{int} = 0.017$
Absorption correction: none	$\theta_{max} = 28.0^\circ$
9248 measured reflections	$h = -17 \rightarrow 13$
1954 independent reflections	$k = -10 \rightarrow 10$
	$l = -19 \rightarrow 19$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0762P)^2 + 0.1221P]$
$R[F^2 > 2\sigma(F^2)] = 0.039$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.105$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.03$	$\Delta\rho_{max} = 0.20$ e Å <sup>-3</sup>
1954 reflections	$\Delta\rho_{min} = -0.24$ e Å <sup>-3</sup>
219 parameters	
H-atom parameters constrained	

**Table 1**

Selected geometric parameters (Å, °).

C1–O1	1.207 (2)	C10–O4	1.448 (2)
C8–O2	1.208 (3)	C16–O3	1.202 (3)
C9–C14	1.339 (3)	C19–O4	1.469 (2)
C16–C11–C12–C13	130.10 (17)	C17–C18–C19–C20	151.45 (18)
C15–C11–C12–C13	-109.02 (19)		

**Table 2**

Hydrogen-bonding geometry (Å, °).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
C5–H5...O1 <sup>i</sup>	0.93	2.55	3.381 (3)	148
C13–H13...O3 <sup>ii</sup>	0.98	2.47	3.268 (3)	138

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

In the absence of anomalous scattering effects, the absolute configuration could not be established in this analysis. Therefore, it was arbitrarily assigned and the Friedel pairs were merged. H atoms were included in calculated positions ( $C-H = 0.93-0.98 \text{ \AA}$ ) using a riding model, with  $U_{iso}$  values set at  $1.2U_{eq}(CH)$  and  $1.5(CH_3)$  times the  $U_{eq}$  values of the parent atoms.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

The authors thank Dr J. S. Yadav, Director of ICT, for his kind encouragement and support.

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