

1,6,6-Trimethyl-1,2,6,7,8,9-hexahydro-phenanthro[1,2-*b*]furan-10,11-dione

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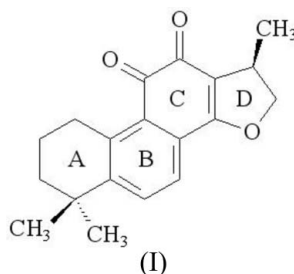
## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
Disorder in main residue  
 $R$  factor = 0.047  
 $wR$  factor = 0.132  
Data-to-parameter ratio = 9.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound,  $\text{C}_{19}\text{H}_{20}\text{O}_3$ , is widely used in China to treat coronary heart diseases. The asymmetric unit contains two independent molecules in which both the five- and the terminal six-membered rings adopt half-chair conformations.

## Comment

The title compound, (I), the main active component isolated from the rhizome of *Salvia miltiorrhiza Bunge* and *Salvia przewalskii Maxim (Labiatae)*, has been used widely in China to treat coronary heart diseases, particularly angina pectoris and myocardial infarction (Xue *et al.*, 1999). We report here the crystal structure of (I).



The asymmetric unit of (I) contains two crystallographically independent molecules (Fig. 1). The corresponding bond lengths of these two molecules agree with each other (Table 1). The C14–C15 and C33–C34 bond distances agree with the corresponding distance of 1.5628 (19) Å reported for 8,9-dihydro-1,6-dimethylphenanthro[1,2-*b*]furan-10,11-dione (Qin *et al.*, 2005). In one of the molecules, the cyclohexene ring *A* is disordered. In both molecules, ring *A* adopts a half-chair conformation and the five-membered ring *D* adopts a distorted half-chair conformation. Intramolecular C–H...O hydrogen bonds are observed in the molecular structure (Table 2), but no intermolecular hydrogen bonding is observed in the crystal structure.

## Experimental

Compound (I) was obtained from the Tasly Group, a pharmaceutical company in Tianjin. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a methanol solution at room temperature.

## Crystal data

$\text{C}_{19}\text{H}_{20}\text{O}_3$   
 $M_r = 296.35$   
Orthorhombic,  $P2_12_12$   
 $a = 14.458$  (3) Å  
 $b = 21.356$  (4) Å  
 $c = 9.874$  (2) Å  
 $V = 3048.7$  (11) Å<sup>3</sup>  
 $Z = 8$   
 $D_x = 1.291$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
Cell parameters from 29524 reflections  
 $\theta = 3.1$ – $27.5^\circ$   
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
Plate, orange  
 $0.67 \times 0.23 \times 0.06$  mm

Data collection

Rigaku R-Axis RAPID IP area-detector diffractometer  
Oscillation scans  
Absorption correction: multi-scan (using intensity measurements) (*ABSCOR*; Higashi, 1995)  
 $T_{\min} = 0.945$ ,  $T_{\max} = 0.995$   
29524 measured reflections

3906 independent reflections  
2348 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.050$   
 $\theta_{\text{max}} = 27.5^\circ$   
 $h = -16 \rightarrow 18$   
 $k = -27 \rightarrow 27$   
 $l = -12 \rightarrow 12$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.132$   
 $S = 0.91$   
3906 reflections  
416 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0861P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.17 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.17 \text{ e } \text{\AA}^{-3}$

Table 1

Selected interatomic distances ( $\text{\AA}$ ).

|        |           |         |           |
|--------|-----------|---------|-----------|
| O1—C12 | 1.346 (4) | O5—C33  | 1.214 (3) |
| O1—C19 | 1.463 (4) | O6—C34  | 1.219 (4) |
| O2—C14 | 1.205 (3) | C12—C16 | 1.339 (4) |
| O3—C15 | 1.226 (3) | C14—C15 | 1.554 (4) |
| O4—C31 | 1.348 (3) | C31—C35 | 1.338 (4) |
| O4—C38 | 1.461 (4) | C33—C34 | 1.557 (4) |

Table 2

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

| $D-H\cdots A$        | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------|-------|-------------|-------------|---------------|
| C6—H6B $\cdots$ O2   | 0.97  | 2.36        | 2.760 (4)   | 104           |
| C25—H25A $\cdots$ O5 | 0.97  | 2.24        | 2.759 (4)   | 113           |
| C29—H29A $\cdots$ O4 | 0.93  | 2.48        | 2.799 (3)   | 100           |

The occupancies of the disordered positions C23/C23' and C24/C24' were refined to 0.646 (13)/0.354 (13). The C—C distances involving the disordered atoms were restrained to 1.52 (1)  $\text{\AA}$ , and the  $U^{ij}$  components of these atoms were approximated to isotropic behaviour. The H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H distances of

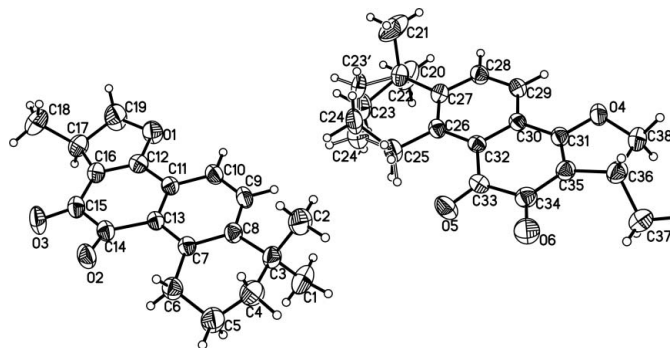


Figure 1

The asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. In one of the molecules, both components of the disordered cyclohexene ring are shown.

0.93–0.98  $\text{\AA}$  [ $U_{\text{iso}}(\text{H})$  values of 1.2 or 1.5 (methyl) times  $U_{\text{eq}}(\text{C})$ ]. However, a short H21B $\cdots$ H23D contact of 1.73  $\text{\AA}$  involving a disordered H atom is observed. In the absence of significant anomalous dispersion effects, Friedel pairs were merged before the final refinement.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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