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1,6-Dimethylphenanthro[1,2-*b*]furan-10,11-dione

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.157
Data-to-parameter ratio = 15.5

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

The title compound, $C_{18}H_{12}O_3$, also known as tanshinone, contains four fused rings. The crystal packing involves offset π-stacking interactions and C—H···O hydrogen bonds.

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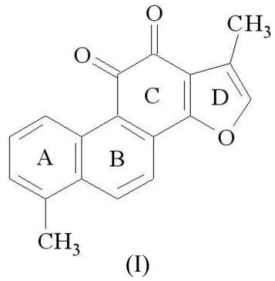
Comment

The title compound, (I), is an active component isolated from the rhizomes of *Salvia Miltiorrhiza Bunge* and *Salvia Przewalskii Maxim* (Labiatae). It is used widely in China to treat coronary heart disease, particularly angina pectoris (Kasimu *et al.*, 1998).



(I)

We report here the structure of (I) (Fig. 1), which has three six-membered rings forming a phenanthrene dione system, with a five-membered methylfuran ring fused to the dione ring. The entire molecule is essentially planar, with a maximum deviation from the least-squares plane through all non-H atoms of 0.369 (2) Å. The structure is similar to that of 1,6,6-trimethyl-1,2,6,7,8,9-hexahydrophenanthro[1,2-*b*]furan-10,11-dione (Zhang *et al.*, 2005), which is another significant active component isolated from the rhizomes of these plants. There are offset π-stacking interactions in the crystal structure, with the planar molecules stacked in a head-to-tail fashion such that the perpendicular distance between rings *A* and *C* in adjacent molecules is 3.706 (3) Å, the distance between rings *B* being 3.773 (3) Å (Fig. 2). Further stabilization results from intermolecular C—H···O hydrogen bonds (Table 1).

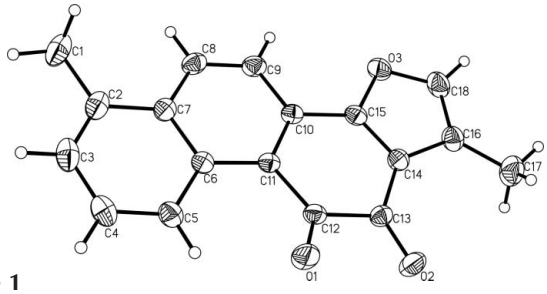


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

Experimental

The title compound was prepared by China's National Institute for the Control of Pharmaceutical and Biological Products from *Salvia Miltiorrhiza Bunge*. The product was characterized by NMR, IR and HPLC. The melting point, determined by differential scanning calorimetry, is 506 K. Red–brown block-shaped single crystals suitable for X-ray diffraction were obtained by slow evaporation of a methanol solution at room temperature.

Crystal data

$C_{18}H_{12}O_3$	$Z = 2$
$M_r = 276.28$	$D_x = 1.411$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.0989$ (14) Å	Cell parameters from 6480 reflections
$b = 7.9539$ (16) Å	$\theta = 3.0$–$27.5°$
$c = 12.162$ (2) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 90.79$ (3)°	$T = 293$ (2) K
$\beta = 105.76$ (3)°	Block, red–brown
$\gamma = 99.65$ (3)°	0.67 × 0.08 × 0.05 mm
$V = 650.3$ (2) Å^3	

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer	2950 independent reflections
	2150 reflections with $I > 2\sigma(I)$
Oscillation scans	$R_{int} = 0.030$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$\theta_{max} = 27.5°$
	$h = -8 \rightarrow 9$
$T_{min} = 0.939$, $T_{max} = 0.995$	$k = -10 \rightarrow 10$
6480 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1061P)^2 + 0.0053P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.046$	
$wR(F^2) = 0.157$	
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
2950 reflections	$\Delta\rho_{max} = 0.19$ e Å^{-3}
190 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1B···O2^{i}	0.96	2.54	3.376 (2)	145
C4—H4A···O1^{ii}	0.93	2.70	3.481 (2)	142

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x, -y, -z$.

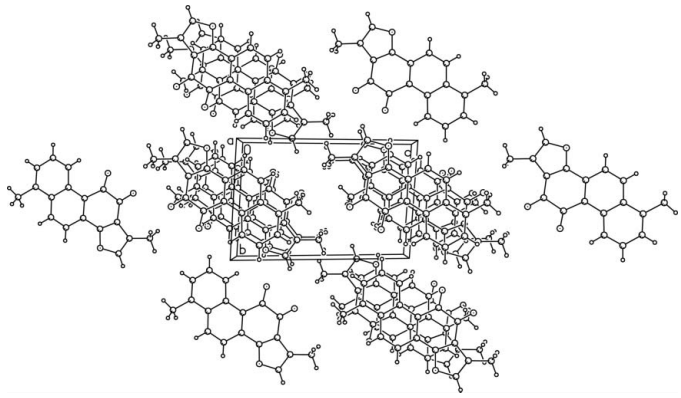


Figure 2
The molecular packing of (I), viewed along the *a* axis.

H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2 (1.5 for Me) times U_{eq}(C).

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: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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