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7-Hydroxy-4,6-dimethyl-3*H*-isobenzofuran-1-one

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.003 Å
R factor = 0.061
wR factor = 0.161
Data-to-parameter ratio = 14.6

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

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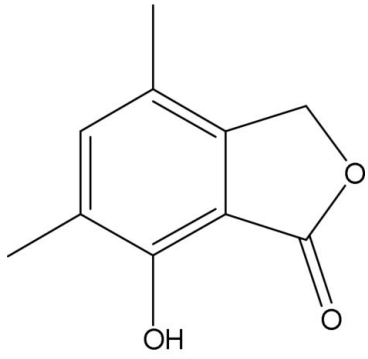
The structure of the title compound, $C_{10}H_{10}O_3$, a colourless lump metabolite isolated from *Diaporthe phaseolorum*, was determined by X-ray analysis. The molecular packing in the crystal structure is stabilized by weak O—H···O═C hydrogen-bonding interactions.

Comment

The title compound, (I), was isolated from *Diaporthe sp*. (see *Experimental*), which grows on the submerged rotten leaves of *kandelia candel* in the mangrove nature conservation areas of Fugong, Fujian Province of China (Lin *et al.*, 2005). In the solid state, compound (I) is a nearly planar molecule, the dihedral angle between the five- and six- membered rings being 1.0 (2)°, a conformation also found in related molecules such as 7-methoxy-4,6-dimethyl-3*H*-isobenzofuran-1-one (Wang *et al.*, 2003).



(I)

Molecules are linked through weak O—H···O═C intermolecular hydrogen bonds, forming centrosymmetric dimers in the crystal structure. Compound (I) exhibits cytotoxicity towards the Raji cell line (IC_{50} = 15 μg ml^{-1}), anti-oxidant activity as a scavenger of 2,2-diphenyl-1,4-phthalazinedione radicals with an IC_{50} value of 61.2 μg ml^{-1}, and moderate activity against *Penicillium avellaneum*, with IC_{50} = 200 μg ml^{-1}.

Experimental

The title compound, (I), was isolated from the organic extract of the agar surface fermentation of *Diaporthe sp*. The strain was grown on modified potato dextrose agar media and extracted with ethyl acetate, which was fractionated by column chromatography over reverse-phase (C-18) Si gel, followed by column chromatography over Si gel and crystallization. Recrystallization from ethyl acetate afforded colourless crystals suitable for X-ray analysis.

Crystal data

$C_{10}H_{10}O_3$	$Z = 8$
$M_r = 178.18$	$D_x = 1.396$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation
$a = 14.362$ (5) Å	$\mu = 0.10$ mm^{-1}
$b = 8.220$ (3) Å	$T = 273$ (2) K
$c = 14.360$ (2) Å	Chunk, colourless
$V = 1695.5$ (9) Å^3	0.38 × 0.25 × 0.11 mm

Data collection

Bruker APEX area-detector diffractometer	8712 measured reflections
φ and ω scans	1750 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	1577 reflections with $I > 2\sigma(I)$
$T_{min} = 0.962$, $T_{max} = 0.989$	$R_{int} = 0.030$
	$\theta_{max} = 26.5°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0779P)^2 + 0.9444P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.061$	$(\Delta/\sigma)_{max} = 0.154$
$wR(F^2) = 0.161$	$\Delta\rho_{max} = 0.27$ e Å^{-3}
$S = 1.11$	$\Delta\rho_{min} = -0.21$ e Å^{-3}
1750 reflections	
120 parameters	
H-atom parameters constrained	

H atoms were positioned geometrically and were included in the refinement in the riding-model approximation, with C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H atoms, respectively, and O—H = 0.82 Å. Isotropic displacement parameters for H atoms were set at U_{iso}(H) = xU_{eq}(carrier atom), with $x = 1.5$ for methyl and hydroxy, and $x = 1.2$ for all other H atoms.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

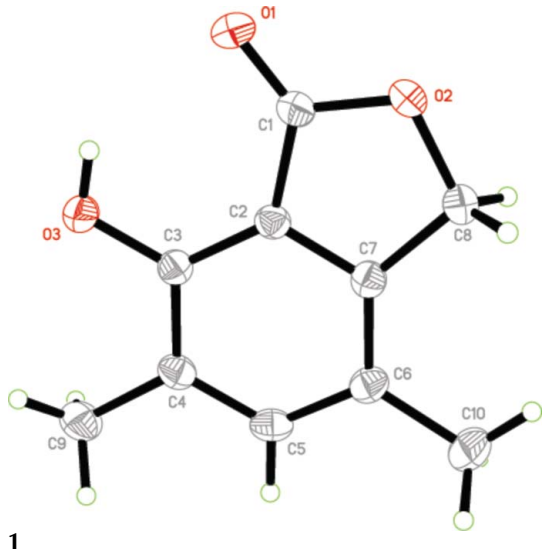


Figure 1
View of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

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