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(*E*)-3-(3-Hydroxy-4-methoxyphenyl)-1-(2-naphthyl)-prop-2-en-1-one

Zhi-Ke Lu,[a,b]* Xue-Min Duan[c] and Peng-Mian Huang[d]

[a]School of Pharmaceuticals & Biotechnology, Tianjin University, Tianjin 300072, People's Republic of China, [b]Forestry College, GuangXi University, Nanning 530005, People's Republic of China, [c]School of Pharmacy, Jiangxi Science & Technology Normal University, Nanchang 330013, People's Republic of China, and [d]School of Chemical & Environmental Engineering, Changsha University of Science & Technology, Changsha 410076, People's Republic of China

Correspondence e-mail: lukz1886@yahoo.com.cn

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The title compound, $C_{20}H_{16}O_3$, was synthesized from 3-hydroxy-4-methoxybenzaldehyde and 2-(prop-1-en-2-yl)-naphthalene in aqueous ethanol. The naphthalene ring system makes a dihedral angle of 15.8 (4) Å with the plane of the benzene ring. In the crystal structure, molecules are linked into centrosymmetric dimers by O—H···O hydrogen bonds.

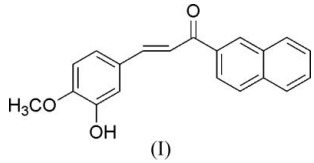
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.056
wR factor = 0.144
Data-to-parameter ratio = 16.3

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

Comment

(*E*)-3-(3-Hydroxy-4-methoxyphenyl1-(2-naphthyl)prop-2-en-1-one, (I), is a valuable pharmaceutical intermediate (Jardine *et al.*, 1980; Issell *et al.*, 1984; Stahelin *et al.*, 1989), which was synthesized by a new method from 3-hydroxy-4-methoxybenzaldehyde and 2-(prop-1-en-2-yl)naphthalene. Its structure is reported here (Fig. 1).



(I)

The dihedral angle formed between the naphthalene ring system and the plane of the benzene ring is 15.8 (4)°. The methoxyl group lies slightly out of the plane of the benzene ring, with atoms O2 and C7 deviating from the C1–C6 ring plane by 0.061 (2) and 0.295 (3) Å, respectively. In the crystal structure, molecules are linked into centrosymmetric dimers by O—H···O hydrogen bonds (Fig. 2 and Table 1).

Experimental

A mixture of 3-hydroxy-4-methoxybenzaldehyde (5 mmol) and 2-(prop-1-en-2-yl)naphthalene (10 mmol) was dissolved in aqueous ethanol (100 ml, 60% *v*/*v*). A solution of KOH (4.0 ml, 7.1 mmol) was added slowly with stirring at 323 K for 5 h. The resulting mixture was neutralized with 2 *M* HCl, the precipitate filtered off, washed with water, and crystallized from dichloromethane–petroleum ether (4:1 *v*/

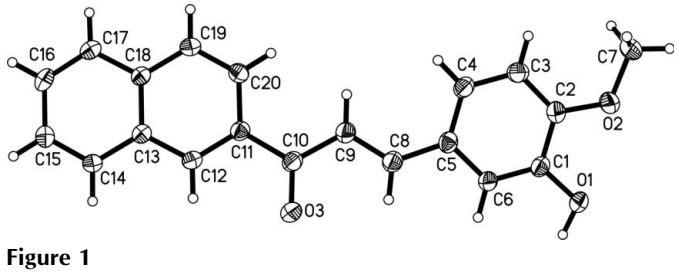


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

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v) to obtain (I) (m.p. 442–443 K). Crystals suitable for X-ray analysis were grown by slow evaporation of a petroleum ether–dichloromethane (4:1 *v*/*v*) solution at room temperature over a period of 17 d.

Crystal data

$C_{20}H_{16}O_3$	$Z = 8$
$M_r = 304.33$	$D_x = 1.360$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation
$a = 14.7417$ (11) Å	$\mu = 0.09$ mm^{-1}
$b = 6.1208$ (4) Å	$T = 293$ (2) K
$c = 32.941$ (3) Å	Prism, colorless
$V = 2972.3$ (4) Å^3	0.22 × 0.16 × 0.14 mm

Data collection

Rigaku Saturn-70 diffractometer	25516 measured reflections
ω scans	3509 independent reflections
Absorption correction: multi-scan (Jacobson, 1998)	3105 reflections with $I > 2\sigma(I)$
$T_{min} = 0.980$, $T_{max} = 0.987$	$R_{int} = 0.058$
	$\theta_{max} = 27.8°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0656P)^2 + 0.9426P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.056$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.144$	$\Delta\rho_{max} = 0.24$ e Å^{-3}
$S = 1.16$	$\Delta\rho_{min} = -0.18$ e Å^{-3}
3509 reflections	Extinction correction: *SHELXL97*
215 parameters	Extinction coefficient: 0.0075 (13)
H atoms treated by a mixture of independent and constrained refinement	

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O3^{i}	0.94 (3)	1.74 (3)	2.6795 (18)	176 (2)

Symmetry code: (i) $-x, -y+1, -z+1$.

The H atom of the OH group was located in a difference Fourier map and refined freely with an isotropic displacement parameter. Other H atoms were included using the riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms.

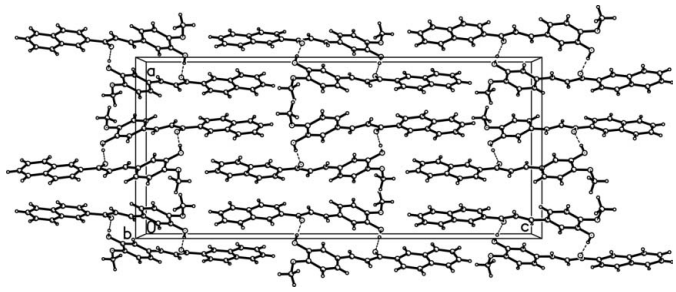

Figure 2
Part of the crystal structure of (I), showing O—H···O hydrogen bonds as dashed lines.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2005).

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