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1-(4-Hydroxyphenyl)-3-(2,4,6-trimethoxyphenyl)propan-1-one

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.076
wR factor = 0.184
Data-to-parameter ratio = 8.6

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

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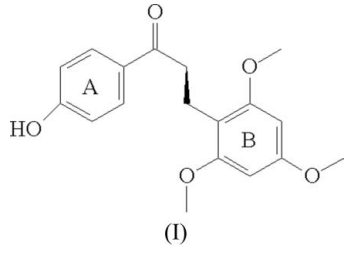
The two benzene rings of the title compound, $C_{18}H_{20}O_5$, are almost parallel, with a dihedral angle of 1.3 (2)°. The hydroxy group forms intermolecular O—H···O hydrogen bonds which link the molecules into infinite chains along the c axis.

Comment

The title compound, (I), also known as loureirin B, was extracted from the herb *Sanguis draxonis* with ethanol (Zhou *et al.*, 2001). The compound was crystallized from methanol: toluene (3:1) and its structure is reported here. The dihedral angle between the planes defined by atoms C1–C6 and C1′–C6′ is 1.3 (2)°. The hydroxyphenyl and trimethoxyphenyl ring planes are separated by 1.414 Å, and the C7═O2 carbonyl group is essentially coplanar with the hydroxyphenyl ring. The hydroxy group forms a strong O—H···O hydrogen bond to the carbonyl O atom, linking the molecules into infinite chains along the c axis.



(I)

Experimental

The title compound was extracted according to the procedure of Zhou *et al.* (2001) from the herb *Sanguis draxonis*. The compound was crystallized from methanol/toluene (3:1), yielding colorless block-like crystals after a week at room temperature.

Crystal data

$C_{18}H_{20}O_5$
M_r = 316.34
Monoclinic, Pc
a = 5.6200 (11) Å
b = 14.447 (3) Å
c = 10.149 (2) Å
β = 96.04 (3)°
V = 819.4 (3) Å^3
Z = 2
D_x = 1.282 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1803 reflections
θ = 4.2–27.2°
μ = 0.09 mm^{-1}
T = 298 (2) K
Block, colorless
0.30 × 0.20 × 0.20 mm

Data collection

MAC DIP 2030K diffractometer
ω scans
Absorption correction: none
3054 measured reflections
1803 independent reflections
1778 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.2°
$h = 0 \rightarrow 7$
$k = -18 \rightarrow 18$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0669P)^2 + 0.3852P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.076$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.184$	$\Delta\rho_{max} = 0.25$ e Å^{-3}
$S = 1.19$	$\Delta\rho_{min} = -0.20$ e Å^{-3}
1803 reflections	Extinction correction: *SHELXL97*
209 parameters	Extinction coefficient: 0.84 (7)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O1—C4	1.347 (6)	C1—C2	1.392 (7)
O2—C7	1.236 (6)	C7—C8	1.498 (7)
O3—C6′	1.366 (6)	C8—C9	1.537 (7)
O3—C7′	1.428 (6)	C9—C1′	1.494 (7)
C6′—O3—C7′	119.2 (4)	C1′—C9—C8	113.2 (4)
C1—C7—C8	120.3 (4)		
O1—C4—C5—C6	−179.1 (5)	C8—C9—C1′—C6′	83.9 (6)
C2—C1—C7—C8	−177.1 (5)	C9′—O5—C2′—C3′	−2.2 (8)
C7—C8—C9—C1′	177.5 (5)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O2^{i}	0.82	1.89	2.708 (5)	179

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

All H atoms were refined using a riding model with C—H = 0.93 Å, U_{iso}(H) = 1.2U_{eq}(C) for aromatic CH; 0.97 Å, U_{iso}(H) = 1.2U_{eq}(C) for CH_2; 0.96 Å, U_{iso}(H) = 1.5U_{eq}(C) for CH_3; and 0.82 Å, U_{iso}(H) = 1.5U_{eq}(O) for OH atoms. In the absence of significant anomalous dispersion effects, Freidel pairs were merged.

Data collection: *DENZO* (Otwinowski & Minor, 1997); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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References

Otwinowski, Z. & Minor, W (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

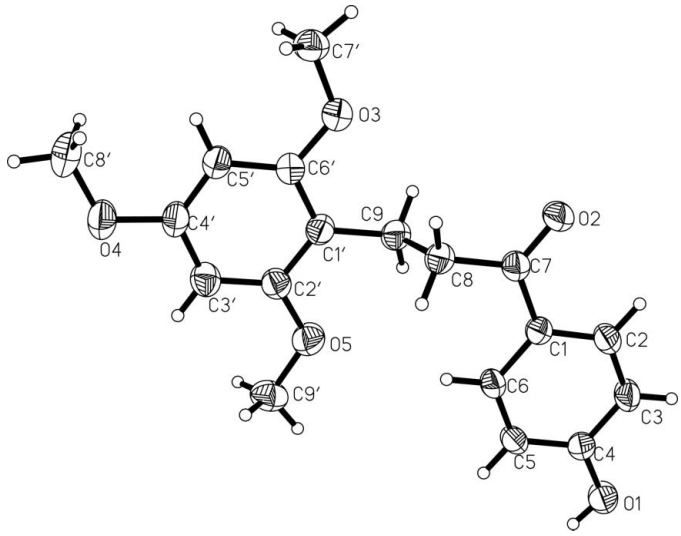

Figure 1
A view of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by circles of arbitrary size.

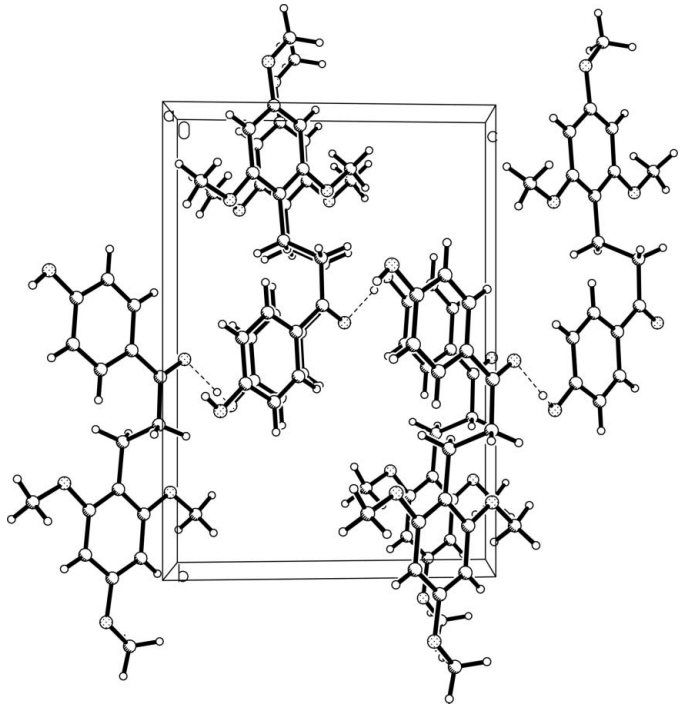

Figure 2
The molecular packing of (I), viewed along the *a* axis. Dashed lines indicate hydrogen-bonding interactions.

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