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5-Hydroxy-7-methoxy-2-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.002 Å
R factor = 0.046
wR factor = 0.128
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.

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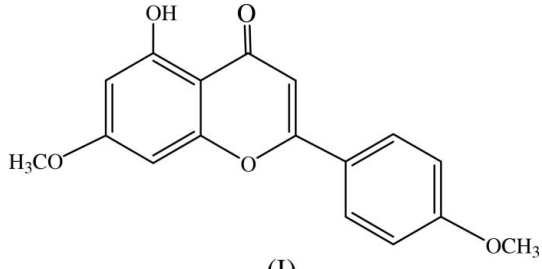
The title compound, $C_{17}H_{14}O_5$, a flavone, was isolated from the rhizomes of *Kaempferia parviflora*. The benzopyran-4-one ring system and the methoxyphenyl substituent are approximately coplanar. The molecules are linked *via* intermolecular C—H···O hydrogen bonds to form chains.

Comment

We have been investigating the compounds present in *Kaempferia parviflora*, a plant growing in the northeastern part of Thailand. Previously, we have reported the isolation and crystal structures of two flavonoids from the rhizomes of this plant (Fun *et al.*, 2005; Teh *et al.*, 2005). The title compound, (I), was also isolated from the rhizomes of *K. parviflora*, which were collected from Loei province in the northeastern part of Thailand. Compound (I), a known flavone, is a secondary metabolite occurring in plants. It does not exhibit antiplasmodium, antifungal, antimycobacterial and cytotoxic activities against KB (oral human epidermoid carcinoma), BC (breast cancer) and NCI-H187 (human small cell lung cancer) cell lines (Yenjai *et al.*, 2004). As part of our ongoing studies on the phytochemistry and biological activities of Thai medicinal plants (Chantrapromma *et al.*, 2003, 2004, 2005; Boonnak *et al.*, 2005; Cheenpracha *et al.*, 2005; Fun *et al.*, 2005; Ng *et al.*, 2005; Pakhathirathien *et al.*, 2005; Teh *et al.*, 2005), we have undertaken the X-ray crystal structure analysis of (I) in order to establish its stereochemistry.



(I)

The bond lengths and angles in (I) (Fig. 1) show normal values (Allen *et al.*, 1987) and are comparable to those observed in 5-hydroxy-3,7-dimethoxy-2-phenyl-4*H*-1-benzopyran-4-one, (II) (Fun *et al.*, 2005), and 3,5,7-trimethoxy-2-phenyl-4*H*-1-benzopyran-4-one, (III) (Teh *et al.*, 2005). Selected bond lengths and angles are given in Table 1. The benzopyran-4-one (C1–C9/O1) ring system is planar within ±0.028 (1) Å. The C1–C9/O1 ring system and C10–C15 benzene ring are approximately coplanar, with a dihedral angle of 7.78 (7)°. The corresponding dihedral angles are 38.00 (3) (molecule *A*) and 13.99 (3)° (molecule *B*) in (II)

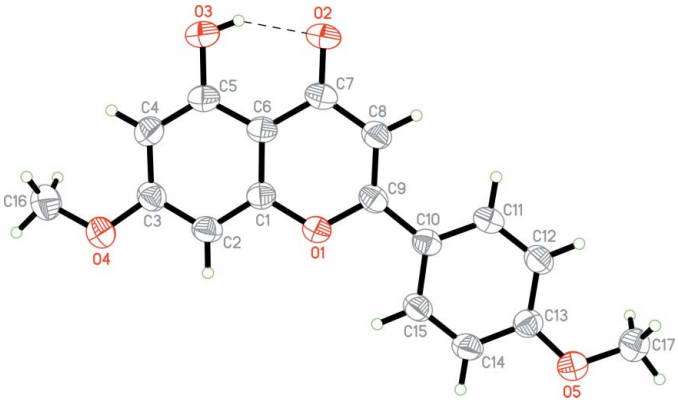


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The dashed line indicates a hydrogen bond.

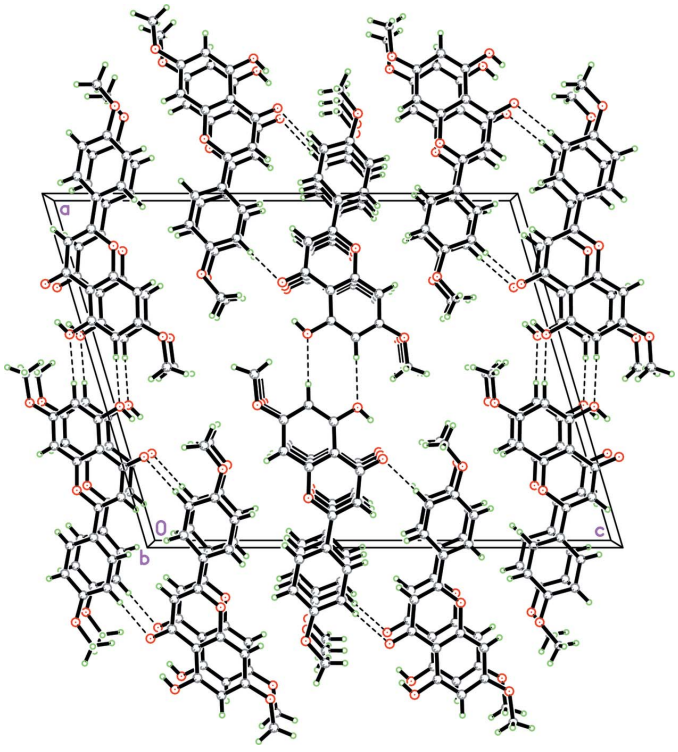


Figure 2
The crystal packing of (I), viewed down the *b* axis, showing hydrogen-bonded (dashed lines) chains.

(Fun *et al.*, 2005), and 31.05 (4)° in (III) (Teh *et al.*, 2005). The two methoxy groups are coplanar with the attached rings.

An intramolecular O—H···O hydrogen bond is observed in the molecular structure (Table 2). Inversion-related molecules are linked by C4—H4···O3^{i} and C12—H12···O2^{ii} (symmetry codes are given in Table 2) hydrogen bonds into a chain along the *a* axis (Fig. 2).

Experimental

Air-dried rhizomes of *K. parviflora* were milled and extracted with hexane and $CHCl_3$ at room temperature. The residue obtained after evaporation of the solvent was separated by quick column chromatography (QCC) over silica gel and eluted with 3% CH_2Cl_2–hexane to afford seven fractions (F1–F7). Fraction F2 was subjected to column chromatography (CC) with 10% acetone–hexane to give five fractions (F2A–F2E). Compound (I) was obtained from fraction F2D. Single crystals of (I) suitable for X-ray diffraction studies were obtained by recrystallization from $CHCl_3$–CH_3OH (4:1 *v*/*v*) after several days (m.p. 447–448 K).

Crystal data

$C_{17}H_{14}O_5$
M_r = 298.28
Monoclinic, $P2_1/c$
a = 16.9406 (4) Å
b = 3.8619 (1) Å
c = 21.7968 (4) Å
β = 106.52 (1)°
V = 1367.15 (9) Å^3
Z = 4
D_x = 1.449 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3581 reflections
θ = 2.0–28.0°
μ = 0.11 mm^{-1}
T = 273 (2) K
Plate, colourless
0.54 × 0.15 × 0.08 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.912, T_{max} = 0.992
17884 measured reflections
3283 independent reflections
2207 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 28.0°
$h = -21 \rightarrow 22$
$k = -5 \rightarrow 5$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.128
S = 1.05
3283 reflections
201 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2 + 0.2601P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C9	1.3645 (17)	O4—C16	1.420 (2)
O1—C1	1.3804 (18)	O5—C13	1.3570 (18)
O2—C7	1.2578 (17)	O5—C17	1.426 (2)
O3—C5	1.3526 (18)	C8—C9	1.354 (2)
O4—C3	1.3652 (19)		
C3—O4—C16	118.12 (14)	C11—C10—C9	121.11 (13)
C13—O5—C17	118.72 (13)		
C16—O4—C3—C2	−171.93 (16)	C17—O5—C13—C12	−3.3 (3)
C16—O4—C3—C4	7.7 (3)	C17—O5—C13—C14	176.77 (16)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2^{i}	0.82	1.83	2.571 (2)	149
C4—H4···O3^{ii}	0.93	2.54	3.441 (2)	163
C12—H12···O2^{iii}	0.93	2.52	3.430 (2)	167

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

H atoms were placed in calculated positions, with O—H = 0.82 Å and C—H = 0.93 or 0.96 Å. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for hydroxy and methyl H atoms, and $1.2U_{eq}$ for the remaining H atoms.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve

structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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5-Hydroxy-7-methoxy-2-(4-methoxyphenyl)-4*H*-1-benzopyran-4-one. Corrigendum

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In the paper by Teh, Fun, Razak, Chantrapromma, Boonnak & Karalai [*Acta Cryst.* (2005), E**61**, o3715–o3717], the data collection temperature is given incorrectly. The correct temperature is given below and in the revised '*Key indicators*'.

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M_r = 298.28
Monoclinic, $P2_1/c$
a = 16.9406 (4) Å
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