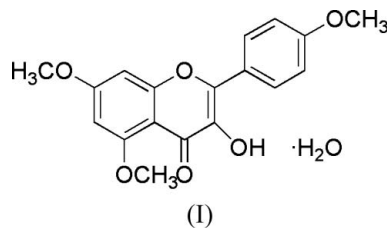


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Key indicators

Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(C-C) = 0.004$ Å
 R factor = 0.053
 wR factor = 0.144
Data-to-parameter ratio = 9.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.3-Hydroxy-5,7,4'-trimethoxyflavone monohydrate
from *Cucubalus baccifer* (L.)The title compound, $C_{18}H_{16}O_6 \cdot H_2O$, is a flavonol which was
isolated from *Cucubalus baccifer* (L.). Intermolecular O—
H \cdots O and C—H \cdots O hydrogen bonds link the molecules to
form networks stacked along the a axis.Received 1 June 2006
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Comment

Cucubalus baccifer (L.) is a Chinese folk herb used for
arthritis, pulmonary tuberculosis (in oral use) and scrofula
(topical use). It is sporadically distributed in northeast,
northwest and southwest China, as well as in Europe, central
Asia and India. Previously, triterpenoids, flavonoids and
phytoecdysterones were isolated from *C. baccifer*. 3-Hydroxy-
5,7,4'-trimethoxyflavone has been isolated from *Aflaia*
(Greger *et al.*, 2001) and from *Alpinia tonkinensi* (Zhang *et al.*,
2003). The chemical structure of the natural product 3-hydroxy-
5,7,4'-trimethoxyflavone from the plants was determined
on the basis of NMR data (Zhang *et al.*, 2003). The chemical
structure of the title monohydrate, (I), has now been
confirmed by single-crystal X-ray diffraction analysis.In the molecule of (I) (Fig. 1), the bond lengths and angles
are within normal ranges (Allen *et al.*, 1987). The rings A (C5–
C10), B (O1/C2–C4/C9/C10) and C (C1'–C6') are each planar,
and they are also nearly coplanar, with a puckering amplitude
of $Q_T = 0.0824$ (3) Å (Cremer & Pople, 1975).As can be seen from the packing diagram (Fig. 2), inter-
molecular O—H \cdots O and C—H \cdots O hydrogen bonds
(Table 1) link the molecules to form networks stacked along
the a axis. Dipole–dipole and van der Waals interactions are
also effective in the molecular packing in the crystal structure.

Experimental

The aerial part of *C. baccifer* was collected in September 2003, in
Hebei province, China. A voucher specimen, identified by Dr Wen-
Yuan Gao, was deposited under registration No. TJU-03928 at the
herbarium of the Department of Natural Products and Traditional
Chinese Medicine, Tianjin University. The material (6 kg) was
refluxed three times with EtOH (95%). The extract was concentrated
under reduced pressure to give a residue (600 g) which was parti-

tioned between ethyl acetate and water (1:1). The EtOAc extract was chromatographed on silica gel column with increasing polarity eluant; similar eluates, as indicated by thin-layer chromatography analysis, were combined to yield 19 fractions. Fraction 2 was subjected to column chromatography on Toyopearl HW-40, eluting with CHCl₃/MeOH (2:1), to yield five fractions. The third fraction was recrystallized from CHCl₃ to afford the title compound, (I) (yield 2.5 g, m.p. 421.2–423.2 K).

Crystal data

C ₁₈ H ₁₆ O ₆ ·H ₂ O	Z = 4
M _r = 346.32	D _x = 1.421 Mg m ⁻³
Orthorhombic, P2 ₁ 2 ₁ 2 ₁	Mo Kα radiation
a = 5.2764 (11) Å	μ = 0.11 mm ⁻¹
b = 11.5152 (18) Å	T = 294 (2) K
c = 26.639 (3) Å	Block, colorless
V = 1618.5 (5) Å ³	0.12 × 0.06 × 0.06 mm

Data collection

Rigaku Saturn 70 diffractometer	12416 measured reflections
ω scans	2246 independent reflections
Absorption correction: multi-scan (Jacobson, 1998)	2035 reflections with I > 2σ(I)
T _{min} = 0.987, T _{max} = 0.993	R _{int} = 0.047
	θ _{max} = 27.8°

Refinement

Refinement on F ²	w = 1/[σ ² (F _o ²) + (0.0696P) ² + 0.1604P]
R[F ² > 2σ(F ²)] = 0.053	where P = (F _o ² + 2F _c ²)/3
wR(F ²) = 0.144	(Δ/σ) _{max} < 0.001
S = 1.21	Δρ _{max} = 0.25 e Å ⁻³
2246 reflections	Δρ _{min} = -0.18 e Å ⁻³
240 parameters	Extinction correction: SHELXL97
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.029 (5)

Table 1

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
O7—H7B...O3 ⁱ	0.91 (5)	2.12 (5)	3.022 (4)	173 (5)
O7—H7A...O3 ⁱⁱ	0.90 (5)	2.04 (5)	2.870 (3)	153 (5)
O2—H2...O3	0.79 (4)	2.18 (4)	2.640 (3)	118 (4)
O2—H2...O7 ⁱⁱⁱ	0.79 (4)	2.03 (4)	2.692 (3)	141 (4)
C2''—H2''3...O6 ^{iv}	0.96	2.55	3.379 (5)	144

Symmetry codes: (i) x + 1, y + 1, z; (ii) x + ½, -y + ½, -z; (iii) x, y - 1, z; (iv) -x + 1, y + ½, -z + ½.

In the absence of significant anomalous dispersion effects, Friedel-pairs were merged prior to refinement. The H atoms of the water molecule and hydroxyl group were located in difference syntheses, and refined, O—H = 0.79 (4)–0.91 (5) Å [*U*_{iso}(H) = 1.5*U*_{eq}(O)]. The remaining H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms with *U*_{iso}(H) = *xU*_{eq}(C), where *x* = 1.2 for aromatic H and *x* = 1.5 for methyl H.

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: *CrystalStructure* (Rigaku/MSC, 2005); software used to prepare material for publication: *CrystalStructure*.

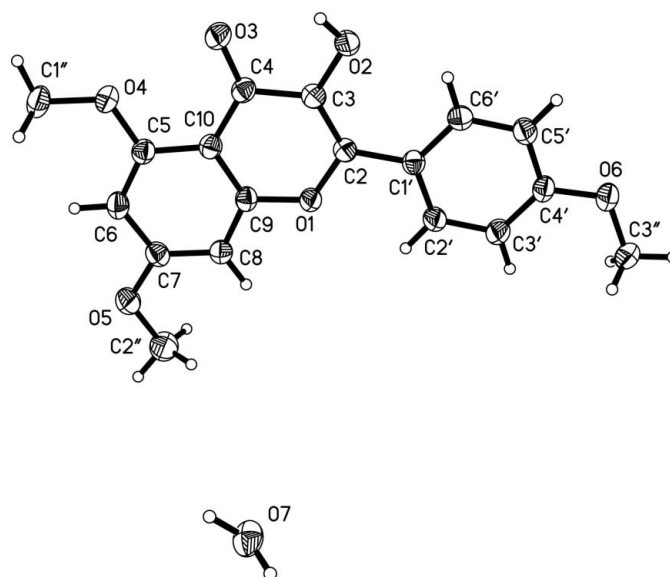


Figure 1
The asymmetric unit, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

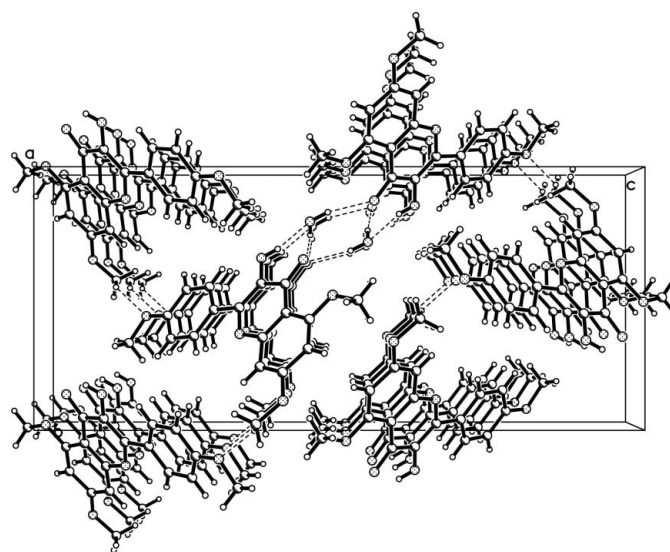


Figure 2
Packing diagram of (I). Intermolecular hydrogen bonds are shown as dashed lines.

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