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5,7-Dihydroxy-8-methoxy-2-phenyl-4*H*-chromen-4-one monohydrate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.054
wR factor = 0.135
Data-to-parameter ratio = 8.8

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

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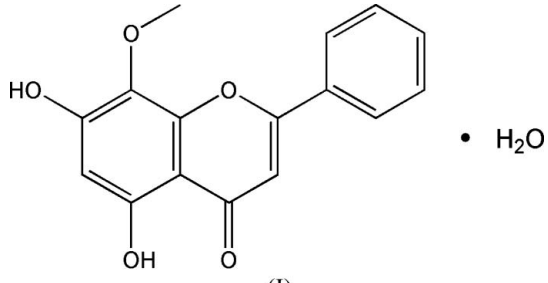
In the crystal structure of the title compound, $C_{16}H_{12}O_5\cdot H_2O$, the water O atom is involved in intermolecular hydrogen bonds which link the molecules into a three-dimensional network.

Comment

The title compound, (I), was extracted from *Scutellaria rehderiana Diels* with acetone (Su *et al.*, 2004; Li & Chen, 2005). Recently, the compound was successfully crystallized from ethyl acetate. The molecule is essentially planar, except for the methoxy methyl group. The dihedral angle between the two benzene rings is 1.5 (2)° and between the C5–C10 and O1/C2/C3/C4/C9/C10 planes is only 0.2 (1)°. The torsion angle O1—C2—C1′—C6′ is −179.8 (3)°.



(I)

Water atom O*W* acts as both a hydrogen-bond acceptor *via* HO4 from the hydroxy group O4 and as a donor *via* atom H*WA* to carbonyl atom O2 of the neighbouring molecule at $(-x-\frac{1}{2}, -y+1, z-\frac{1}{2})$, as well as with the neighbouring O*W* atom at $(x+\frac{1}{2}, -y+\frac{1}{2}, -z)$.

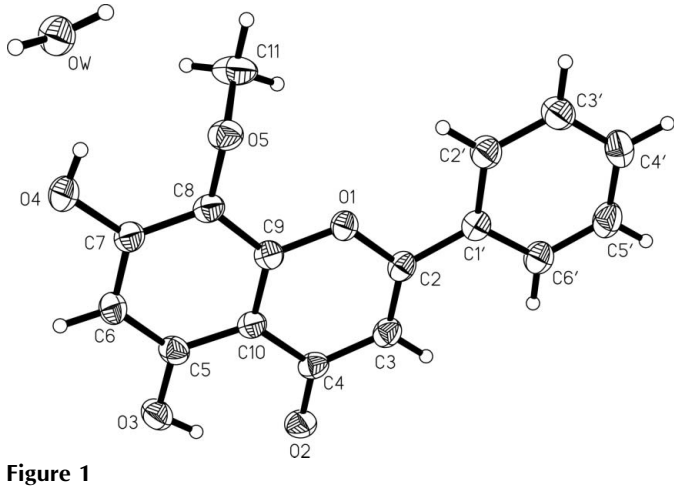


Figure 1
The asymmetric unit of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by circles of arbitrary size.

The interaction of atoms O3 with O2 is intramolecular and completes a closed six-membered ring. Water molecules link to form chains which, in turn, link the chromenone molecules, forming a hydrogen-bonded three-dimensional network.

Experimental

The title compound was prepared according to the procedure for extracting *Scutellaria rehderiana Diels* (Su *et al.*, 2004; Li & Chen, 2005). At 283 K and under unventilated conditions, crystals appropriate for data collection were obtained by evaporation of an ethyl acetate solution over a period of one week.

Crystal data

$C_{16}H_{12}O_5\cdot H_2O$
$M_r = 302.27$
Orthorhombic, $P2_12_12_1$
$a = 4.7160$ (9) Å
$b = 16.551$ (3) Å
$c = 18.466$ (4) Å
$V = 1441.4$ (5) Å^3
$Z = 4$
$D_x = 1.393$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1825 reflections
$\theta = 3.5$–27.3°
$\mu = 0.11$ mm^{-1}
$T = 298$ (2) K
Prism, yellow
0.40 × 0.10 × 0.10 mm

Data collection

MAC DIP 2030K diffractometer
ω scans
Absorption correction: none
4404 measured reflections
1825 independent reflections
1801 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 27.3°$
$h = 0 \rightarrow 5$
$k = -21 \rightarrow 21$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.135$
$S = 1.23$
1825 reflections
208 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 0.6551P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.059 (11)

Table 1
Selected geometric parameters (Å, °).

O2—C4	1.262 (4)	C9—C10	1.401 (4)
C2—C1′	1.466 (4)	C1′—C2′	1.394 (5)
C5—C6	1.378 (4)	C4′—C5′	1.383 (5)
C6—C7	1.398 (5)		
C2—O1—C9	119.6 (2)	C5—C6—C7	119.6 (3)
C8—O5—C11	113.4 (3)	C2′—C1′—C2	121.4 (3)
C3—C2—O1	121.7 (3)	C2′—C3′—C4′	120.1 (4)
C11—O5—C8—C9	83.0 (4)	O1—C2—C1′—C2′	−0.3 (4)
C2—O1—C9—C8	−179.5 (3)	O1—C2—C1′—C6′	−179.8 (3)
C3—C2—C1′—C2′	178.5 (4)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O2	0.82	1.88	2.609 (3)	147
O4—H4A···OW	0.82	2.02	2.766 (4)	151
OW—HWA···O2^{i}	0.90 (5)	1.93 (5)	2.828 (3)	177 (5)
OW—HWB···OW^{ii}	0.90 (9)	2.03 (8)	2.903 (3)	161 (7)

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

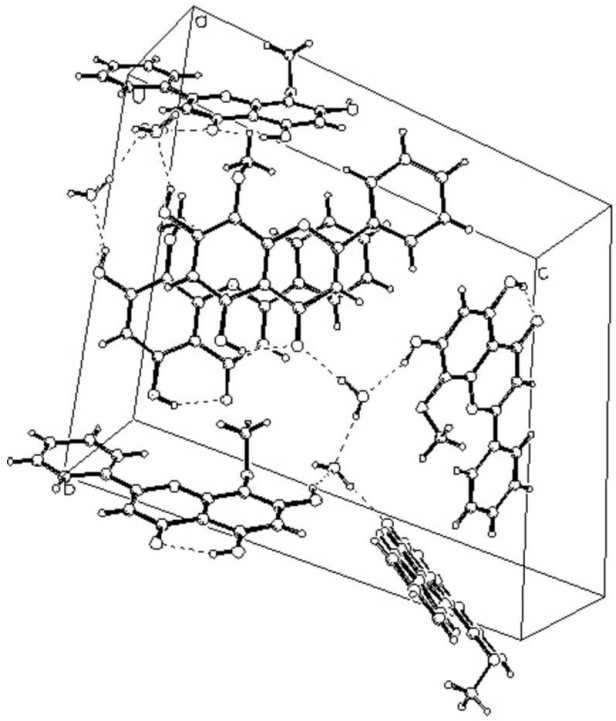


Figure 2
The molecular packing of the title compound. Dashed lines indicate the hydrogen-bonding interactions.

Water H atoms were initially located in a difference Fourier map and refined freely. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.92–0.98 Å and O—H distances of 0.82 Å and with U_{iso}(H) = 1.2 or 1.5 times (for methyl H) U_{eq}(C) and $1.5U_{eq}$(O). In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

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: *ORTEPII* (Johnson, 1976) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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