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# 5,7-Dihydroxy-3,6-dimethoxy-2-(4-methoxyphenyl)-4*H*-chromen-4-one monohydrate

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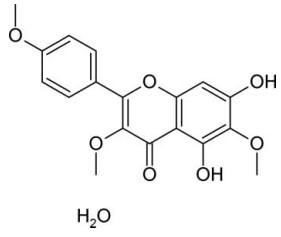
Key indicators: single-crystal X-ray study; $T$ = 150 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.050; $wR$ factor = 0.142; data-to-parameter ratio = 14.0.

The title compound, $C_{18}H_{16}O_7\cdot H_2O$, is a flavonoid isolated from *Dodonaea viscosa*. The benzopyran ring system of the flavonoid is essentially planar [maximum deviation = 0.025 (2) Å] and inclined at 5.83 (2)° to the attached benzene ring. The water of hydration is involved in extensive hydrogen bonding, assembling the molecules into a supramolecular network *via* classical intermolecular O—H···O hydrogen bonding. The crystal structure is further stabilized by $\pi$–$\pi$ stacking interactions [centroid–centroid distance between benzene rings = 3.564 (3) Å].

## Related literature

For the anti-oxidant activity of flavonoids, see: Pedrielli *et al.* (2001, for their anti-protozoal activity, see: Calzada *et al.* (1999) and for their anti-viral activity, see: Lin *et al.* (1999). For hydrogen-bond motifs, see: Etter *et al.* (1990). For related structures, see: Arfan *et al.* (2010); Azhar ul *et al.* (2004); Ferheen *et al.* (2005); Hussain *et al.* (2008, 2009); Jan *et al.* (2009); Khan *et al.* (2005*a*,*b*); Nisar *et al.* (2010); Riaz *et al.* (2002); Sharif *et al.* (2005).




## Experimental

### Crystal data

$C_{18}H_{16}O_7\cdot H_2O$
$M_r$ = 362.32
Monoclinic, $C2/c$
$a$ = 19.869 (4) Å
$b$ = 6.8126 (15) Å
$c$ = 24.424 (5) Å
$\beta$ = 91.298 (4)°
$V$ = 3305.2 (12) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.12 mm$^{-1}$
$T$ = 150 K
0.19 × 0.18 × 0.09 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008*a*)
$T_{min}$ = 0.978, $T_{max}$ = 0.990
14127 measured reflections
3400 independent reflections
2072 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.068

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.142
$S$ = 1.05
3400 reflections
243 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.28 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2*A*···O1*W*$^{i}$ | 0.84 | 1.92 | 2.712 (3) | 157 |
| O2—H2*A*···O3 | 0.84 | 2.33 | 2.780 (3) | 114 |
| O4—H4*A*···O5 | 0.84 | 1.85 | 2.589 (3) | 146 |
| O1*W*—H1*A*···O5 | 0.85 (2) | 2.05 (2) | 2.886 (3) | 165 (3) |
| O1*W*—H1*A*···O6 | 0.85 (2) | 2.71 (3) | 3.288 (3) | 126 (3) |
| O1*W*—H1*B*···O4$^{ii}$ | 0.86 (2) | 2.38 (2) | 3.135 (3) | 148 (3) |

Symmetry codes: (i) $x-\frac{1}{2}, y-\frac{1}{2}, z$; (ii) $-x+\frac{3}{2}, -y+\frac{1}{2}, -z+1$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008*b*); molecular graphics: *SHELXTL* (Sheldrick, 2008*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2231).

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# supplementary materials

*Acta Cryst.* (2010). E**66**, o2716-o2717 [ **doi:10.1107/S1600536810039012** ]

# 5,7-Dihydroxy-3,6-dimethoxy-2-(4-methoxyphenyl)-4*H*-chromen-4-one monohydrate

**A. Mohammad, I. Anis, V. McKee, J. W. A. Frese and M. R. Shah**

## Comment

Our investigation on natural product chemistry (Arfan *et al.*, (2010); Azhar *et al.*, (2004); Ferheen *et al.*, (2005); Hussain *et al.*, (2008, 2009); Jan *et al.*, 2009) is intended to explore the medicinal aspect of indigenous plants (Khan *et al.*, (2005*a*); Khan *et al.*, (2005*b*); Nisar *et al.*, (2010); Riaz *et al.*, (2002); Sharif *et al.*, (2005).) of Pakistan. The plant *Dodonaea Viscosa* has been screened for the presence of biologically active compounds resulting in the isolation of a Flavonoid (Fig.1). The crystal structure and isolation of the title compound are presented below. Flavonoids, comprising a vast family of polyphenolic secondary metabolites, exhibit a wide range of biological activities, such as anti–oxidant (Pedrielli *et al.*, 2001), anti–viral (Lin *et al.*, 1999), anti–protozoal (Calzada, *et al.,* 1999).

The methoxy groups at C4 and C9 of title compound (Fig. 1) are nearly orthogonal to the benzopyranone moiety, as indicated by the torsion angles 97.5 (3)° and 107.6 (3)° respectively. The methoxy group at C15 is nearly coplanar with the phenyl ring with torsion angle (C17–C15–O7–C16) 0.3 (4)°. Rings *A* and *B* (the benzopyrone moiety) are fused at C1 and C7 and almost coplanar, the interplanar angle between the two rings is 1.40 (3)°. Ring *C* (the phenyl moeity) is attached to benzopyranone system at C11 with an interplanar angle of 5.83 (2)° between the two ring systems.

A combination of intermolecular and intramolecular hydrogen bonding, forming $R^4_6(12)$ and $R^4_4(16)$ patterns (Etter *et al.*, 1990), links the molecules into stepped ribbons perpendicular to *b* axis (Fig. 2 and Table 1). The ribbons are stacked parallel to the *b* axis by π–π interactions (Fig. 3); the average interplanar distance is 3.378 (3)Å (under symmetry operation 3/2-x, -1/2+y, 3/2-z) and the distance from the centroid of the phenyl group to the centre of the C1–C7 bond is 3.476 (3)Å.

## Experimental

The whole plant of *Dodonaea viscosa* (50 kg) was powdered and extracted with methanol (100 L × 3) at room temperature and the residue (1 kg) was separated under vacuum. The residue was suspended in water and extracted with *n*–hexane, chloroform, ethyl acetate and *n*–butanol respectively. The ethyl acetate fraction (250 g) was subjected repeatedly to column chromatography on silica gel using petroleum ether with a gradient of 25% chloroform to yield the title compound (50 mg). Single crystals suitable for X–ray diffraction analysis were obtained from an ether–chloroform mixture (1:2) by slow evaporation of the solvent at room temperature.

## Refinement

H atoms bonded to carbon and the phenol oxygen atoms were placed in geometric positions using a riding model, C—H distances were constrained as 0.95Å, 0.98Å and 0.84Å, for aryl, methyl and phenol groups respectively. Hydrogen atoms on the water molecule were located from difference maps and their coordinates refined under restraints. Thermal parameters were set to $U_{iso}$(H) = 1.5$U_{eq}$(C, O) for methyl groups and the water molecule and $U_{iso}$(H) = 1.2$U_{eq}$(C) for all others.

**Figures**

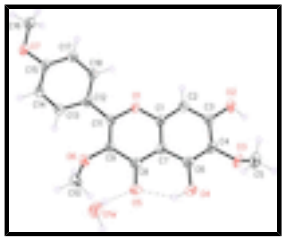

Fig. 1. Molecular structure of title compound with atom numbering scheme. Displacement ellipsoids are drawn at 50% probability level. H atoms are presented as a small spheres of arbitrary radius. Several H bonds are drawn by dashed lines.

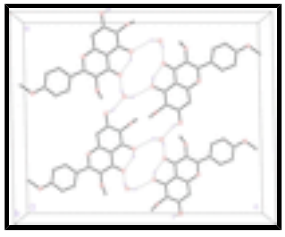

Fig. 2. Packing diagram showing the H–bond network (dashed lines).

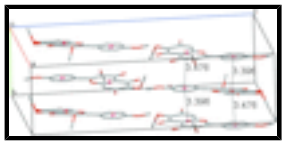

Fig. 3. The π–π interactions. Red cirles mark centroids of bonds or rings.

**5,7-Dihydroxy-3,6-dimethoxy-2-(4-methoxyphenyl)-4*H*-chromen-4-one monohydrate**

*Crystal data*

| | |
|---|---|
| $C_{18}H_{16}O_7 \cdot H_2O$ | $F(000) = 1520$ |
| $M_r = 362.32$ | $D_x = 1.456$ Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation, λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 1391 reflections |
| *a* = 19.869 (4) Å | θ = 2.6–22.0° |
| *b* = 6.8126 (15) Å | μ = 0.12 mm$^{-1}$ |
| *c* = 24.424 (5) Å | *T* = 150 K |
| β = 91.298 (4)° | Block, yellow |
| *V* = 3305.2 (12) Å$^3$ | 0.19 × 0.18 × 0.09 mm |
| *Z* = 8 | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 3400 independent reflections |
| Radiation source: fine–focus sealed tube | 2072 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.068$ |
| φ and ω scans | $\theta_{max} = 26.4°$, $\theta_{min} = 1.7°$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008*a*) | *h* = −24→24 |
| $T_{min} = 0.978$, $T_{max} = 0.990$ | *k* = −8→8 |
| 14127 measured reflections | *l* = −30→30 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.050$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.142$ | H atoms treated by a mixture of independent and constrained refinement |
| $S = 1.05$ | $w = 1/[\sigma^2(F_o^2) + (0.0597P)^2 + 1.2286P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 3400 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 243 parameters | $\Delta\rho_{max} = 0.28$ e Å$^{-3}$ |
| 3 restraints | $\Delta\rho_{min} = -0.28$ e Å$^{-3}$ |

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*–factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*–factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*–factors(gt) etc. and is not relevant to the choice of reflections for refinement. *R*–factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*–factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.69131 (8) | 0.1125 (2) | 0.73867 (6) | 0.0233 (4) |
| C1 | 0.65171 (12) | 0.1096 (4) | 0.69190 (10) | 0.0229 (6) |
| C2 | 0.58358 (12) | 0.0898 (4) | 0.69845 (10) | 0.0258 (6) |
| H2 | 0.5651 | 0.0824 | 0.7339 | 0.031* |
| C3 | 0.54256 (13) | 0.0807 (4) | 0.65176 (10) | 0.0263 (6) |
| O2 | 0.47576 (9) | 0.0548 (3) | 0.65803 (8) | 0.0367 (5) |
| H2A | 0.4573 | 0.0329 | 0.6274 | 0.063 (11)* |
| C4 | 0.56984 (13) | 0.0955 (4) | 0.59938 (10) | 0.0268 (6) |
| O3 | 0.52807 (9) | 0.0810 (2) | 0.55366 (7) | 0.0313 (5) |
| C5 | 0.50843 (15) | 0.2684 (4) | 0.53157 (11) | 0.0381 (7) |
| H5A | 0.4789 | 0.2488 | 0.4993 | 0.057* |
| H5B | 0.5486 | 0.3413 | 0.5210 | 0.057* |
| H5C | 0.4844 | 0.3429 | 0.5593 | 0.057* |
| C6 | 0.63836 (13) | 0.1158 (4) | 0.59382 (10) | 0.0248 (6) |
| O4 | 0.66442 (10) | 0.1283 (3) | 0.54307 (7) | 0.0326 (5) |
| H4A | 0.7066 | 0.1279 | 0.5456 | 0.079 (13)* |
| C7 | 0.68135 (12) | 0.1217 (4) | 0.64058 (9) | 0.0223 (5) |

| | | | | |
|---|---|---|---|---|
| C8 | 0.75264 (12) | 0.1433 (4) | 0.63673 (10) | 0.0236 (6) |
| O5 | 0.78120 (9) | 0.1632 (3) | 0.59130 (7) | 0.0314 (5) |
| C9 | 0.79061 (12) | 0.1419 (4) | 0.68777 (10) | 0.0230 (6) |
| O6 | 0.85888 (8) | 0.1730 (3) | 0.68523 (7) | 0.0308 (5) |
| C10 | 0.89618 (14) | 0.0038 (5) | 0.66731 (12) | 0.0463 (8) |
| H10A | 0.9442 | 0.0360 | 0.6666 | 0.069* |
| H10B | 0.8805 | −0.0341 | 0.6305 | 0.069* |
| H10C | 0.8892 | −0.1054 | 0.6927 | 0.069* |
| C11 | 0.75982 (12) | 0.1256 (4) | 0.73687 (10) | 0.0227 (6) |
| C12 | 0.79011 (12) | 0.1236 (3) | 0.79246 (10) | 0.0216 (5) |
| C13 | 0.85991 (12) | 0.1219 (4) | 0.80250 (10) | 0.0264 (6) |
| H13 | 0.8895 | 0.1229 | 0.7725 | 0.032* |
| C14 | 0.88602 (13) | 0.1188 (4) | 0.85496 (10) | 0.0253 (6) |
| H14 | 0.9334 | 0.1153 | 0.8609 | 0.030* |
| C15 | 0.84399 (12) | 0.1208 (4) | 0.89942 (10) | 0.0225 (5) |
| O7 | 0.87539 (8) | 0.1210 (3) | 0.94962 (7) | 0.0300 (4) |
| C16 | 0.83423 (14) | 0.1220 (5) | 0.99661 (10) | 0.0407 (7) |
| H16A | 0.8629 | 0.1224 | 1.0298 | 0.061* |
| H16B | 0.8057 | 0.0047 | 0.9963 | 0.061* |
| H16C | 0.8058 | 0.2396 | 0.9960 | 0.061* |
| C17 | 0.77463 (12) | 0.1225 (4) | 0.89071 (10) | 0.0252 (6) |
| H17 | 0.7453 | 0.1239 | 0.9209 | 0.030* |
| C18 | 0.74882 (12) | 0.1220 (4) | 0.83780 (10) | 0.0232 (6) |
| H18 | 0.7014 | 0.1206 | 0.8321 | 0.028* |
| O1W | 0.88745 (11) | 0.4465 (4) | 0.57732 (8) | 0.0492 (6) |
| H1A | 0.8602 (15) | 0.357 (4) | 0.5866 (12) | 0.074* |
| H1B | 0.8908 (17) | 0.435 (5) | 0.5425 (7) | 0.074* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0190 (9) | 0.0306 (10) | 0.0200 (9) | −0.0011 (7) | −0.0033 (7) | −0.0012 (8) |
| C1 | 0.0253 (13) | 0.0201 (13) | 0.0230 (13) | 0.0015 (10) | −0.0049 (11) | −0.0001 (11) |
| C2 | 0.0245 (14) | 0.0287 (15) | 0.0243 (13) | 0.0006 (11) | 0.0005 (11) | −0.0022 (11) |
| C3 | 0.0240 (14) | 0.0253 (15) | 0.0294 (14) | −0.0005 (11) | −0.0028 (11) | −0.0007 (11) |
| O2 | 0.0221 (10) | 0.0538 (14) | 0.0340 (11) | −0.0035 (9) | −0.0051 (8) | −0.0030 (9) |
| C4 | 0.0340 (15) | 0.0214 (14) | 0.0246 (14) | 0.0005 (11) | −0.0076 (11) | −0.0029 (11) |
| O3 | 0.0352 (11) | 0.0284 (10) | 0.0297 (10) | −0.0006 (8) | −0.0143 (8) | −0.0011 (8) |
| C5 | 0.0397 (17) | 0.0334 (17) | 0.0405 (17) | 0.0053 (13) | −0.0154 (13) | 0.0020 (13) |
| C6 | 0.0314 (15) | 0.0206 (13) | 0.0223 (13) | 0.0029 (11) | −0.0003 (11) | −0.0013 (11) |
| O4 | 0.0339 (12) | 0.0423 (12) | 0.0217 (10) | 0.0024 (9) | −0.0011 (8) | −0.0005 (8) |
| C7 | 0.0260 (13) | 0.0190 (13) | 0.0219 (13) | 0.0025 (11) | −0.0018 (10) | −0.0010 (10) |
| C8 | 0.0277 (14) | 0.0206 (13) | 0.0226 (13) | 0.0014 (11) | 0.0029 (11) | −0.0005 (10) |
| O5 | 0.0288 (10) | 0.0439 (12) | 0.0217 (10) | 0.0000 (9) | 0.0026 (8) | 0.0000 (8) |
| C9 | 0.0191 (13) | 0.0246 (14) | 0.0253 (13) | −0.0010 (10) | 0.0012 (10) | −0.0005 (11) |
| O6 | 0.0211 (9) | 0.0428 (12) | 0.0285 (10) | −0.0036 (8) | 0.0024 (8) | 0.0014 (8) |
| C10 | 0.0263 (16) | 0.072 (2) | 0.0404 (17) | 0.0160 (15) | 0.0009 (13) | −0.0118 (16) |
| C11 | 0.0189 (13) | 0.0216 (13) | 0.0276 (14) | 0.0014 (10) | −0.0004 (11) | −0.0009 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C12 | 0.0229 (13) | 0.0181 (13) | 0.0238 (13) | −0.0001 (10) | −0.0028 (10) | −0.0014 (10) |
| C13 | 0.0236 (13) | 0.0291 (14) | 0.0267 (14) | −0.0003 (11) | 0.0013 (11) | −0.0012 (12) |
| C14 | 0.0216 (13) | 0.0264 (14) | 0.0278 (14) | 0.0005 (11) | −0.0027 (11) | 0.0016 (11) |
| C15 | 0.0245 (13) | 0.0189 (13) | 0.0239 (13) | −0.0004 (10) | −0.0027 (11) | −0.0003 (10) |
| O7 | 0.0262 (10) | 0.0426 (11) | 0.0211 (9) | 0.0009 (8) | −0.0041 (7) | 0.0002 (8) |
| C16 | 0.0323 (16) | 0.068 (2) | 0.0211 (14) | −0.0006 (15) | −0.0012 (12) | 0.0013 (14) |
| C17 | 0.0249 (14) | 0.0281 (14) | 0.0228 (13) | 0.0010 (11) | 0.0016 (11) | −0.0008 (11) |
| C18 | 0.0207 (13) | 0.0242 (13) | 0.0246 (13) | −0.0001 (11) | −0.0005 (10) | −0.0011 (11) |
| O1W | 0.0424 (13) | 0.0714 (17) | 0.0334 (12) | −0.0225 (11) | −0.0046 (10) | 0.0037 (11) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C11 | 1.366 (3) | O6—C10 | 1.444 (3) |
| O1—C1 | 1.372 (3) | C10—H10A | 0.9800 |
| C1—C2 | 1.373 (3) | C10—H10B | 0.9800 |
| C1—C7 | 1.399 (3) | C10—H10C | 0.9800 |
| C2—C3 | 1.388 (3) | C11—C12 | 1.473 (3) |
| C2—H2 | 0.9500 | C12—C18 | 1.393 (3) |
| C3—O2 | 1.351 (3) | C12—C13 | 1.403 (3) |
| C3—C4 | 1.404 (4) | C13—C14 | 1.372 (3) |
| O2—H2A | 0.8400 | C13—H13 | 0.9500 |
| C4—C6 | 1.378 (4) | C14—C15 | 1.385 (3) |
| C4—O3 | 1.380 (3) | C14—H14 | 0.9500 |
| O3—C5 | 1.436 (3) | C15—O7 | 1.363 (3) |
| C5—H5A | 0.9800 | C15—C17 | 1.390 (3) |
| C5—H5B | 0.9800 | O7—C16 | 1.424 (3) |
| C5—H5C | 0.9800 | C16—H16A | 0.9800 |
| C6—O4 | 1.357 (3) | C16—H16B | 0.9800 |
| C6—C7 | 1.411 (3) | C16—H16C | 0.9800 |
| O4—H4A | 0.8400 | C17—C18 | 1.379 (3) |
| C7—C8 | 1.429 (3) | C17—H17 | 0.9500 |
| C8—O5 | 1.265 (3) | C18—H18 | 0.9500 |
| C8—C9 | 1.442 (3) | O1W—H1A | 0.852 (17) |
| C9—C11 | 1.363 (3) | O1W—H1B | 0.859 (17) |
| C9—O6 | 1.376 (3) | | |
| C11—O1—C1 | 121.81 (19) | O6—C10—H10A | 109.5 |
| O1—C1—C2 | 116.9 (2) | O6—C10—H10B | 109.5 |
| O1—C1—C7 | 120.0 (2) | H10A—C10—H10B | 109.5 |
| C2—C1—C7 | 123.1 (2) | O6—C10—H10C | 109.5 |
| C1—C2—C3 | 118.1 (2) | H10A—C10—H10C | 109.5 |
| C1—C2—H2 | 121.0 | H10B—C10—H10C | 109.5 |
| C3—C2—H2 | 121.0 | C9—C11—O1 | 120.1 (2) |
| O2—C3—C2 | 118.2 (2) | C9—C11—C12 | 129.0 (2) |
| O2—C3—C4 | 120.9 (2) | O1—C11—C12 | 110.9 (2) |
| C2—C3—C4 | 120.9 (2) | C18—C12—C13 | 117.3 (2) |
| C3—O2—H2A | 109.5 | C18—C12—C11 | 119.8 (2) |
| C6—C4—O3 | 120.3 (2) | C13—C12—C11 | 122.9 (2) |
| C6—C4—C3 | 120.0 (2) | C14—C13—C12 | 121.0 (2) |
| O3—C4—C3 | 119.7 (2) | C14—C13—H13 | 119.5 |

| | | | |
|---|---|---|---|
| C4—O3—C5 | 113.20 (19) | C12—C13—H13 | 119.5 |
| O3—C5—H5A | 109.5 | C13—C14—C15 | 120.7 (2) |
| O3—C5—H5B | 109.5 | C13—C14—H14 | 119.7 |
| H5A—C5—H5B | 109.5 | C15—C14—H14 | 119.7 |
| O3—C5—H5C | 109.5 | O7—C15—C14 | 115.7 (2) |
| H5A—C5—H5C | 109.5 | O7—C15—C17 | 124.7 (2) |
| H5B—C5—H5C | 109.5 | C14—C15—C17 | 119.6 (2) |
| O4—C6—C4 | 119.6 (2) | C15—O7—C16 | 117.7 (2) |
| O4—C6—C7 | 120.1 (2) | O7—C16—H16A | 109.5 |
| C4—C6—C7 | 120.3 (2) | O7—C16—H16B | 109.5 |
| C6—O4—H4A | 109.5 | H16A—C16—H16B | 109.5 |
| C1—C7—C6 | 117.6 (2) | O7—C16—H16C | 109.5 |
| C1—C7—C8 | 120.2 (2) | H16A—C16—H16C | 109.5 |
| C6—C7—C8 | 122.2 (2) | H16B—C16—H16C | 109.5 |
| O5—C8—C7 | 122.3 (2) | C18—C17—C15 | 119.3 (2) |
| O5—C8—C9 | 121.5 (2) | C18—C17—H17 | 120.3 |
| C7—C8—C9 | 116.2 (2) | C15—C17—H17 | 120.3 |
| C11—C9—O6 | 121.0 (2) | C17—C18—C12 | 122.1 (2) |
| C11—C9—C8 | 121.6 (2) | C17—C18—H18 | 118.9 |
| O6—C9—C8 | 117.2 (2) | C12—C18—H18 | 118.9 |
| C9—O6—C10 | 113.8 (2) | H1A—O1W—H1B | 105 (2) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2A···O1W$^{i}$ | 0.84 | 1.92 | 2.712 (3) | 157 |
| O2—H2A···O3 | 0.84 | 2.33 | 2.780 (3) | 114 |
| O4—H4A···O5 | 0.84 | 1.85 | 2.589 (3) | 146 |
| O1W—H1A···O5 | 0.85 (2) | 2.05 (2) | 2.886 (3) | 165 (3) |
| O1W—H1A···O6 | 0.85 (2) | 2.71 (3) | 3.288 (3) | 126 (3) |
| O1W—H1B···O4$^{ii}$ | 0.86 (2) | 2.38 (2) | 3.135 (3) | 148 (3) |

Symmetry codes: (i) $x-1/2$, $y-1/2$, $z$; (ii) $-x+3/2$, $-y+1/2$, $-z+1$.

**Fig. 1**

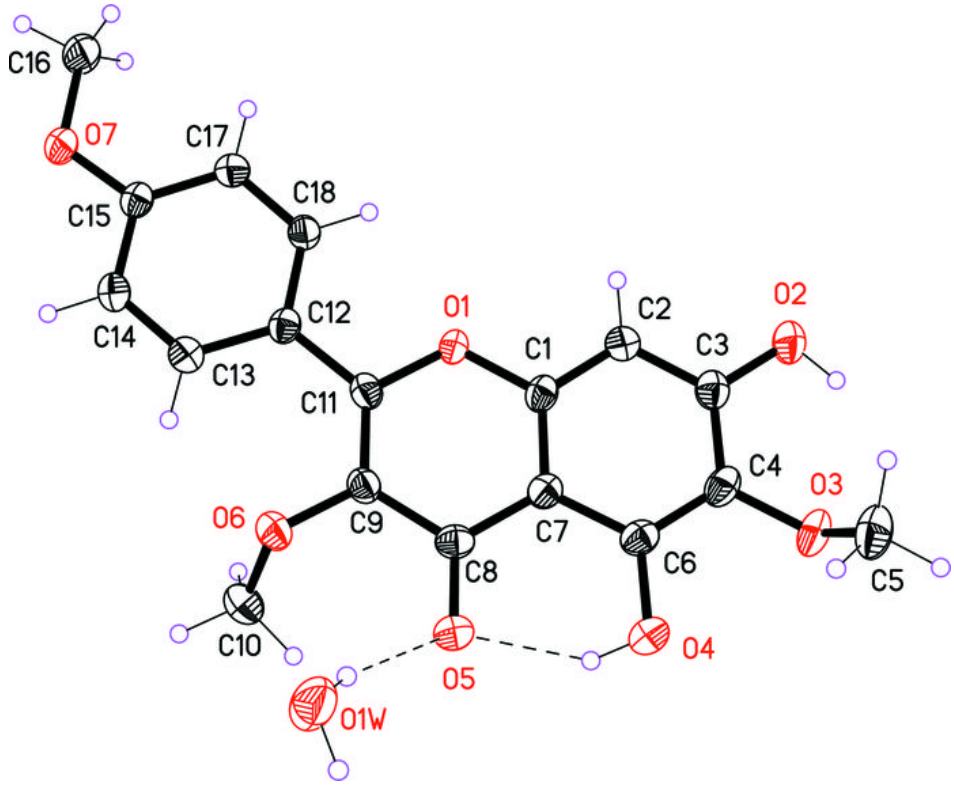
C16
O7
C17
C18
C15
C14
C12
O1
C2
O2
C1
C3
C13
C11
C4
O3
O6
C9
C7
C6
C8
C5
C10
O5
O4
O1W

**Fig. 2**

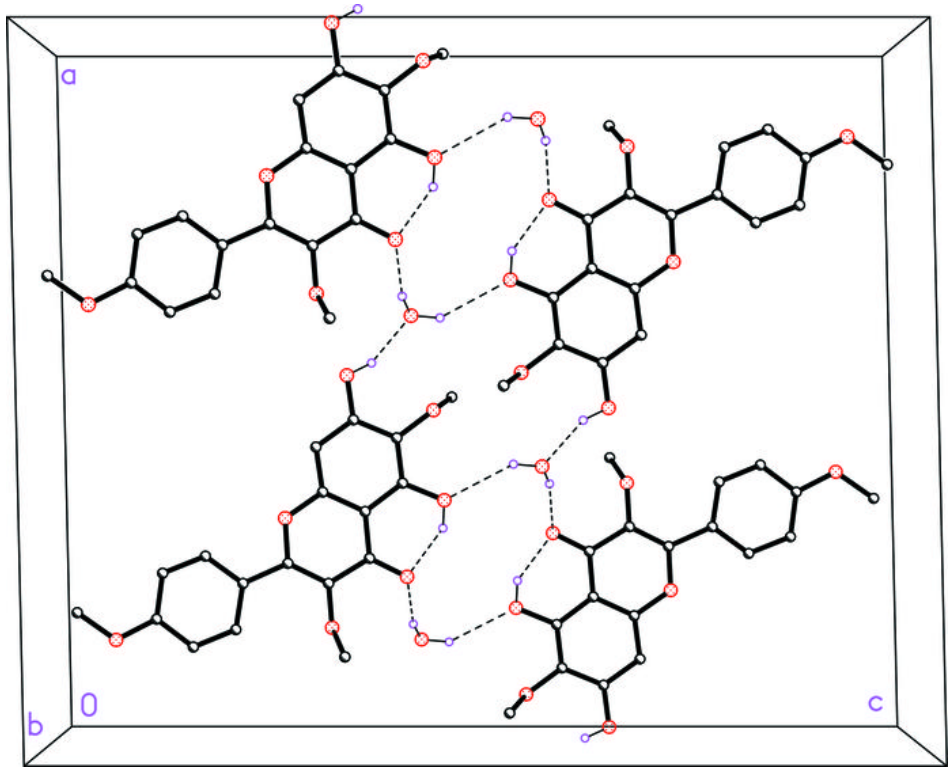

**Fig. 3**