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5-Hydroxy-2-phenyl-7-(prop-2-yn-1-yloxy)-4*H*-chromen-4-one

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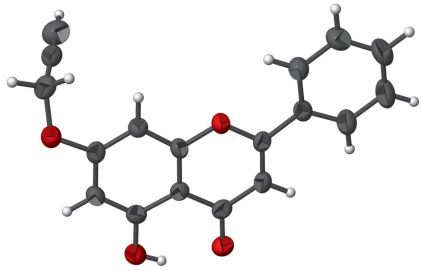
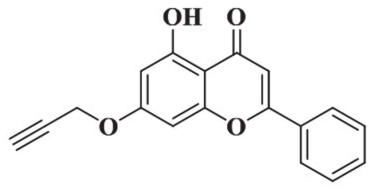
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{18}H_{12}O_4$, the essentially planar chromenone ring system [the maximum deviation = 0.016 (2) Å] is nearly co-planar with the phenyl ring [dihedral angle = 3.85 (8)°]. An intramolecular O—H···O hydrogen bond occurs. In the crystal, weak C—H···O hydrogen bonds and π–π stacking interactions link the molecules into a three-dimensional supramolecular network.

3D view



Chemical scheme



Structure description

Chrysin (5,7-dihydroxy-2-phenyl-4*H*-chromen-4-one) is usually extracted from the passion flower and from honeycomb (Sun *et al.*, 2012). It has the characteristics of flavonoids (Wang *et al.*, 2014). Chrysin has been confirmed to possess pharmacological effects including anti-diarrhoeal, anti-carcinogenic and anti-inflammatory activities (Yang *et al.*, 2014; Ronnekleiv-Kelly *et al.*, 2016; Rauf *et al.*, 2015). Thus, the modification of chrysin is of interest in flavonoid research.

The title compound is similar to its chrysin precursor, which contains three aromatic ring moieties, except for the replacement of hydrogen by an alkynyl group (Fig. 1). The carbonyl C═O bond length is 1.263 (2) Å, while the other C—O bonds are in the range 1.357 (2) to 1.433 (2) Å. The C17—C18 bond length is 1.165 (3) Å, indicating that the alkynyl group has successfully replaced the hydroxy hydrogen atom of the chrysin precursor. The essentially planar chromenone ring system [maximum deviation = 0.016 (2) Å] is nearly co-planar with the phenyl ring [dihedral angle = 3.85 (8)°]. An intramolecular O1—H1*A*···O2 hydrogen bond occurs (Table 1).

In the crystal, weak C—H···O hydrogen bonds (Table 1) and π–π interactions [centroid–centroid distances $Cg1\cdots Cg3(1-x, 1-y, 1-z)$ = 3.6071 (12) Å and $Cg2\cdots Cg3(1-x, 1-y, 1-z)$ = 3.8933 (12) Å; $Cg1$, $Cg2$ and $Cg3$ are the centroids of the

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O2	0.82	1.85	2.584 (2)	148
C3—H3···O2^{i}	0.93	2.48	3.408 (2)	177
C18—H18···O2^{ii}	0.93	2.45	3.330 (3)	157

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

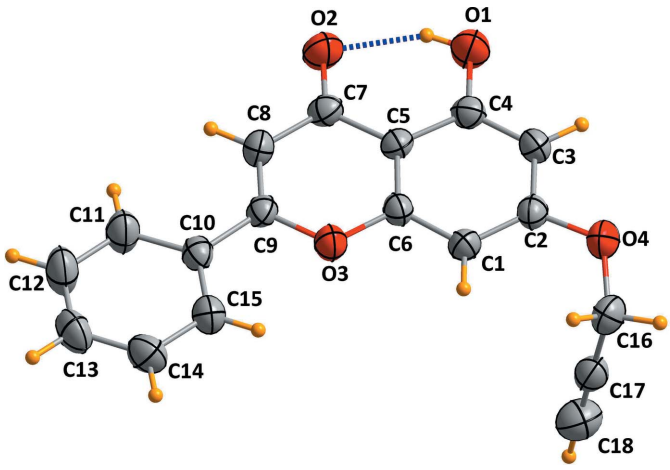


Figure 1
The molecular structure of the title compound. The dashed line indicates the intramolecular hydrogen bond.

O1/C5–C9, C1–C6 and C10–C15 rings, respectively] link the molecules into a three-dimensional supramolecular network.

A search of the Cambridge Structural Database (Groom *et al.*, 2016) revealed the structure of a related compound, 5,7-dihydroxy-3,6-dimethoxy-2-(4-methoxyphenyl)-4*H*-chromen-4-one monohydrate (Mohammad *et al.*, 2010), in which the 4-hydroxyl group of chrysin is replaced by a 3-bromopropyne group.

Synthesis and crystallization

A mixture of chrysin (5 mmol, 1.23 g) and K_2CO_3 (10 mmol, 1.38 g) in acetone (20 ml) stirred at 353 K until the solids were dissolved completely. Then 3-bromo-1-propyne (7.5 mmol, 0.89 g) was added dropwise to the above solution. The mixture was stirred under reflux for 6 h. Colourless bipyramidal crystals were obtained from an acetone solution after 3 d by slow evaporation of the solvent at room temperature.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The data collection was performed at the College of Phamacy, Jiamusi University.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{12}O_4$
M_r	292
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	295
a, b, c (Å)	7.2074 (10), 13.1851 (15), 14.848 (2)
β (°)	102.505 (14)
V (Å^3)	1377.5 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.1 × 0.08 × 0.06
Data collection	
Diffractometer	Agilent New Gemini, Dual, Cu at zero, EosS2
Absorption correction	Multi-scan (SCALE3 ABSPACK in *CrysAlis PRO*; Agilent, 2015)
T_{min}, T_{max}	0.992, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8328, 2715, 1659
R_{int}	0.041
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.111, 0.98
No. of reflections	2715
No. of parameters	199
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.15, −0.17

Computer programs: *CrysAlis PRO* (Agilent, 2015), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *DIAMOND* (Brandenburg & Berndt, 1999).

Funding information

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full crystallographic data

IUCrData (2017). **2**, x170490 [https://doi.org/10.1107/S2414314617004904]

5-Hydroxy-2-phenyl-7-(prop-2-yn-1-yloxy)-4*H*-chromen-4-one

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5-Hydroxy-2-phenyl-7-(prop-2-yn-1-yloxy)-4*H*-chromen-4-one

Crystal data

$C_{18}H_{12}O_4$
M_r = 292
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 7.2074 (10) Å
b = 13.1851 (15) Å
c = 14.848 (2) Å
β = 102.505 (14)°
V = 1377.5 (3) Å^3
Z = 4
$F(000)$ = 608
D_x = 1.409 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1686 reflections
θ = 3.8–26.5°
μ = 0.10 mm^{-1}
T = 295 K
Bipyramid, colorless
0.1 × 0.08 × 0.06 mm

Data collection

Agilent New Gemini, Dual, Cu at zero, EosS2 diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1280 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (SCALE3 ABSPACK in CrysAlisPro; Agilent, 2015)
T_{min} = 0.992, T_{max} = 1.000
8328 measured reflections
2715 independent reflections
1659 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 26.0°, θ_{min} = 3.5°
h = −8→6
k = −16→15
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.111
S = 0.98
2715 reflections
199 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Special details

Experimental. Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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.
H atoms were placed in calculated positions and refined in riding mode, $U_{iso}(H) = 1.5U_{eq}(O)$ for the hydroxyl-H atom and $1.2_{eq}(C)$ for the others.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.6978 (3)	0.75602 (14)	0.64191 (13)	0.0385 (5)
H1	0.8083	0.7546	0.6192	0.046*
C2	0.6296 (3)	0.84539 (14)	0.67119 (12)	0.0373 (5)
C3	0.4655 (3)	0.84843 (14)	0.70599 (12)	0.0392 (5)
H3	0.4242	0.9095	0.7262	0.047*
C4	0.3653 (3)	0.76160 (14)	0.71045 (13)	0.0374 (5)
C5	0.4284 (3)	0.66764 (13)	0.68123 (12)	0.0333 (5)
C6	0.5947 (3)	0.66882 (13)	0.64792 (12)	0.0346 (5)
C7	0.3272 (3)	0.57441 (14)	0.68426 (12)	0.0374 (5)
C8	0.4111 (3)	0.48605 (14)	0.65360 (12)	0.0387 (5)
H8	0.3515	0.4237	0.6549	0.046*
C9	0.5730 (3)	0.49037 (13)	0.62307 (12)	0.0342 (5)
C10	0.6740 (3)	0.40468 (14)	0.59232 (12)	0.0352 (5)
C11	0.5985 (3)	0.30727 (15)	0.58787 (15)	0.0517 (6)
H11	0.4826	0.2964	0.6043	0.062*
C12	0.6929 (3)	0.22674 (17)	0.55946 (16)	0.0610 (7)
H12	0.6401	0.1621	0.5567	0.073*
C13	0.8633 (3)	0.24088 (16)	0.53535 (15)	0.0554 (6)
H13	0.9267	0.1860	0.5165	0.066*
C14	0.9411 (3)	0.33648 (16)	0.53894 (14)	0.0535 (6)
H14	1.0567	0.3464	0.5221	0.064*
C15	0.8473 (3)	0.41805 (15)	0.56767 (13)	0.0448 (5)
H15	0.9011	0.4824	0.5704	0.054*
C16	0.8636 (3)	0.94818 (16)	0.62002 (14)	0.0479 (5)
H16A	0.9563	0.8945	0.6379	0.057*
H16B	0.9278	1.0126	0.6354	0.057*
C17	0.7874 (3)	0.94335 (15)	0.52047 (16)	0.0454 (5)
C18	0.7235 (3)	0.94124 (17)	0.44139 (19)	0.0636 (7)
H18	0.6726	0.9396	0.3783	0.076*
O1	0.20205 (19)	0.76456 (10)	0.74190 (10)	0.0533 (4)
H1A	0.1573	0.7073	0.7408	0.080*
O2	0.17536 (19)	0.57122 (10)	0.71351 (10)	0.0512 (4)

O3	0.66511 (17)	0.58021 (9)	0.61863 (9)	0.0401 (4)
O4	0.71629 (19)	0.93772 (9)	0.67054 (9)	0.0475 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0406 (11)	0.0334 (11)	0.0450 (12)	−0.0040 (9)	0.0172 (10)	−0.0026 (9)
C2	0.0455 (12)	0.0302 (11)	0.0353 (11)	−0.0048 (9)	0.0068 (10)	−0.0017 (8)
C3	0.0479 (12)	0.0327 (11)	0.0399 (11)	0.0037 (10)	0.0158 (10)	−0.0032 (9)
C4	0.0389 (11)	0.0386 (12)	0.0367 (11)	0.0045 (10)	0.0125 (10)	0.0030 (9)
C5	0.0365 (11)	0.0331 (11)	0.0307 (10)	0.0002 (9)	0.0084 (9)	0.0026 (8)
C6	0.0413 (11)	0.0281 (11)	0.0349 (10)	0.0037 (9)	0.0095 (9)	−0.0014 (8)
C7	0.0383 (12)	0.0379 (12)	0.0370 (11)	0.0020 (10)	0.0102 (9)	0.0074 (9)
C8	0.0448 (12)	0.0287 (11)	0.0431 (11)	−0.0023 (9)	0.0105 (10)	0.0010 (9)
C9	0.0405 (11)	0.0288 (11)	0.0328 (10)	0.0003 (9)	0.0069 (9)	0.0037 (8)
C10	0.0403 (11)	0.0313 (11)	0.0324 (10)	0.0044 (9)	0.0046 (9)	0.0020 (8)
C11	0.0508 (13)	0.0354 (13)	0.0715 (15)	0.0001 (11)	0.0191 (12)	−0.0036 (11)
C12	0.0649 (16)	0.0341 (13)	0.0852 (18)	0.0014 (12)	0.0191 (14)	−0.0098 (12)
C13	0.0633 (15)	0.0417 (14)	0.0615 (15)	0.0150 (12)	0.0145 (13)	−0.0073 (11)
C14	0.0526 (14)	0.0535 (15)	0.0584 (14)	0.0083 (12)	0.0211 (12)	−0.0032 (11)
C15	0.0520 (13)	0.0349 (12)	0.0492 (12)	0.0008 (10)	0.0147 (11)	−0.0021 (9)
C16	0.0514 (13)	0.0402 (12)	0.0538 (13)	−0.0102 (10)	0.0151 (11)	0.0003 (10)
C17	0.0468 (13)	0.0370 (12)	0.0563 (15)	0.0000 (10)	0.0198 (12)	0.0039 (10)
C18	0.0658 (16)	0.0688 (18)	0.0575 (16)	−0.0028 (13)	0.0162 (14)	0.0067 (13)
O1	0.0519 (9)	0.0429 (8)	0.0748 (10)	0.0028 (7)	0.0349 (8)	−0.0012 (7)
O2	0.0487 (9)	0.0451 (9)	0.0679 (10)	−0.0033 (7)	0.0308 (8)	0.0017 (7)
O3	0.0431 (8)	0.0298 (8)	0.0517 (8)	−0.0002 (6)	0.0198 (7)	−0.0020 (6)
O4	0.0603 (9)	0.0340 (8)	0.0538 (9)	−0.0106 (7)	0.0242 (7)	−0.0084 (6)

Geometric parameters (Å, º)

C1—C6	1.382 (2)	C10—C15	1.387 (3)
C1—C2	1.383 (2)	C10—C11	1.391 (3)
C1—H1	0.9300	C11—C12	1.376 (3)
C2—O4	1.369 (2)	C11—H11	0.9300
C2—C3	1.390 (2)	C12—C13	1.365 (3)
C3—C4	1.363 (2)	C12—H12	0.9300
C3—H3	0.9300	C13—C14	1.376 (3)
C4—O1	1.357 (2)	C13—H13	0.9300
C4—C5	1.419 (2)	C14—C15	1.386 (3)
C5—C6	1.392 (2)	C14—H14	0.9300
C5—C7	1.435 (2)	C15—H15	0.9300
C6—O3	1.381 (2)	C16—O4	1.433 (2)
C7—O2	1.263 (2)	C16—C17	1.463 (3)
C7—C8	1.432 (2)	C16—H16A	0.9700
C8—C9	1.341 (2)	C16—H16B	0.9700
C8—H8	0.9300	C17—C18	1.165 (3)
C9—O3	1.367 (2)	C18—H18	0.9300

C9—C10	1.469 (2)	O1—H1A	0.8200
C6—C1—C2	117.11 (18)	C15—C10—C9	121.30 (17)
C6—C1—H1	121.4	C11—C10—C9	120.63 (18)
C2—C1—H1	121.4	C12—C11—C10	120.8 (2)
O4—C2—C1	124.15 (18)	C12—C11—H11	119.6
O4—C2—C3	113.79 (16)	C10—C11—H11	119.6
C1—C2—C3	122.05 (18)	C13—C12—C11	120.5 (2)
C4—C3—C2	119.73 (18)	C13—C12—H12	119.7
C4—C3—H3	120.1	C11—C12—H12	119.7
C2—C3—H3	120.1	C12—C13—C14	119.8 (2)
O1—C4—C3	120.01 (17)	C12—C13—H13	120.1
O1—C4—C5	119.27 (17)	C14—C13—H13	120.1
C3—C4—C5	120.71 (18)	C13—C14—C15	120.1 (2)
C6—C5—C4	117.12 (17)	C13—C14—H14	120.0
C6—C5—C7	120.20 (17)	C15—C14—H14	120.0
C4—C5—C7	122.67 (17)	C14—C15—C10	120.65 (19)
O3—C6—C1	116.35 (17)	C14—C15—H15	119.7
O3—C6—C5	120.38 (16)	C10—C15—H15	119.7
C1—C6—C5	123.27 (17)	O4—C16—C17	111.47 (16)
O2—C7—C8	122.65 (17)	O4—C16—H16A	109.3
O2—C7—C5	121.57 (17)	C17—C16—H16A	109.3
C8—C7—C5	115.78 (17)	O4—C16—H16B	109.3
C9—C8—C7	122.08 (18)	C17—C16—H16B	109.3
C9—C8—H8	119.0	H16A—C16—H16B	108.0
C7—C8—H8	119.0	C18—C17—C16	178.4 (2)
C8—C9—O3	121.36 (17)	C17—C18—H18	180.0
C8—C9—C10	126.74 (18)	C4—O1—H1A	109.5
O3—C9—C10	111.89 (16)	C9—O3—C6	120.17 (15)
C15—C10—C11	118.07 (18)	C2—O4—C16	118.70 (15)
C6—C1—C2—O4	179.29 (17)	C7—C8—C9—O3	−0.8 (3)
C6—C1—C2—C3	0.5 (3)	C7—C8—C9—C10	178.32 (16)
O4—C2—C3—C4	179.98 (17)	C8—C9—C10—C15	−175.85 (18)
C1—C2—C3—C4	−1.1 (3)	O3—C9—C10—C15	3.4 (2)
C2—C3—C4—O1	−178.12 (16)	C8—C9—C10—C11	3.6 (3)
C2—C3—C4—C5	1.0 (3)	O3—C9—C10—C11	−177.13 (17)
O1—C4—C5—C6	178.83 (16)	C15—C10—C11—C12	−0.2 (3)
C3—C4—C5—C6	−0.3 (3)	C9—C10—C11—C12	−179.75 (18)
O1—C4—C5—C7	−0.6 (3)	C10—C11—C12—C13	0.2 (3)
C3—C4—C5—C7	−179.72 (18)	C11—C12—C13—C14	−0.4 (3)
C2—C1—C6—O3	−179.84 (15)	C12—C13—C14—C15	0.5 (3)
C2—C1—C6—C5	0.2 (3)	C13—C14—C15—C10	−0.5 (3)
C4—C5—C6—O3	179.72 (15)	C11—C10—C15—C14	0.4 (3)
C7—C5—C6—O3	−0.8 (3)	C9—C10—C15—C14	179.90 (17)
C4—C5—C6—C1	−0.3 (3)	C8—C9—O3—C6	1.6 (3)
C7—C5—C6—C1	179.11 (17)	C10—C9—O3—C6	−177.70 (14)
C6—C5—C7—O2	−179.50 (17)	C1—C6—O3—C9	179.34 (16)

C4—C5—C7—O2	−0.1 (3)	C5—C6—O3—C9	−0.7 (2)
C6—C5—C7—C8	1.5 (3)	C1—C2—O4—C16	13.3 (3)
C4—C5—C7—C8	−179.10 (16)	C3—C2—O4—C16	−167.81 (15)
O2—C7—C8—C9	−179.68 (17)	C17—C16—O4—C2	70.0 (2)
C5—C7—C8—C9	−0.7 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O2	0.82	1.85	2.584 (2)	148
C3—H3···O2^{i}	0.93	2.48	3.408 (2)	177
C18—H18···O2^{ii}	0.93	2.45	3.330 (3)	157

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