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1-(4-Hydroxyphenyl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one

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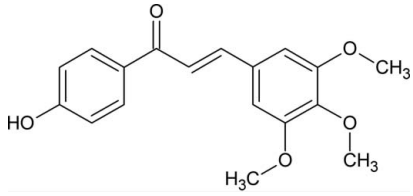
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.066; wR factor = 0.179; data-to-parameter ratio = 14.6.

In the chalcone-derived title compound, $C_{18}H_{18}O_5$, the dihedral angle between the aromatic ring mean planes is 16.64 (15)°. In the crystal structure, adjacent molecules interact by way of O—H···O=C hydrogen bonds, leading to $C(8)$ chains. A C—H···π interaction also helps to stabilize the centrosymmetric crystal packing.

Related literature

For related chalcone derivatives with different substituents at the 4-hydroxy position, see: Teh *et al.* (2006); Ng, Patil *et al.* (2006); Ng, Razak, Fun, Patil, Dharmaprakash & Shettigar (2006); Ng, Razak, Fun, Patil & Dharmaprakash (2006). For the 2-hydroxy isomer of the title compound, which coincidentally possesses a very similar unit cell, see Wu *et al.* (2005).

For other relevant literature see: Butcher *et al.* (2006); Harrison *et al.* (2006); Indira *et al.* (2002); Kiran *et al.* (2007); Patil *et al.* (2006); Uchida *et al.* (1998); Vogel (1999); Zhao *et al.* (2000).



Experimental

Crystal data

$C_{18}H_{18}O_5$
M_r = 314.32
Monoclinic, $P2_1/c$
a = 12.4431 (18) Å
b = 8.5528 (12) Å
c = 15.470 (2) Å
β = 106.399 (2)°
V = 1579.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 295 (2) K
0.25 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.960, T_{max} = 0.981
7097 measured reflections
3088 independent reflections
1656 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.179
S = 1.00
3088 reflections
211 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

*Cg*1 is the centroid of the C10–C15 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.93	1.83	2.660 (3)	147
C2—H2···*Cg*1^{ii}	0.93	2.72	3.536 (3)	147

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2015).

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supplementary materials

Acta Cryst. (2007). E**63**, o2928 [**doi:10.1107/S1600536807024038**]

1-(4-Hydroxyphenyl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one

W. T. A. Harrison, V. Kumari, H. J. Ravindra and S. M. Dharmaprakash

Comment

Organic nonlinear optical materials derived from chalcone are attractive due to their large second harmonic conversion efficiency and excellent blue light transmission (Harrison *et al.*,. 2006; Butcher *et al.*,. 2006; Zhao *et al.*,. 2000). These chalcones crystallize in a non-centrosymmetric crystal structure and provide a necessary configuration for NLO activity with two aromatic rings connected through a conjugated chian (Uchida *et al.*, 1998; Indira *et al.*, 2002.). The chalcone molecules also show good third order nonlinear response (Kiran *et al.* 2007). The nonlinear refractive index of the title compound was measured to be of the order 10^{-11} esu. With this background and also to better understand the structure—nonlinear optical property relationship for this family of compounds, the single-crystal X-ray diffraction study of the title compound, (I) has been carried out.

The molecular structure of (I) is shown in Fig. 1. The bond lengths and angles for (I) are comparable with related molecules such as 1-(4-chlorophenyl) −3-(2,4,5-trimethoxyphenyl)-prop-2-en-1-one (Patil *et al.*,. 2006), and 1-phenyl-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one (Teh *et al.*,. 2006). The C12 and C14 methoxy groups are coplanar with the attached C10—C15 benzene ring with C11—C12—O3—C16 and C15—C14—O5—C18 torsion angles of −3.3 (4)° and 2.1 (4)°, respectively. The other (C13) methoxy group is twisted away form the C10—C15 ring, with a C12—C13—O4—C17 torsion angle of −79.7 (3)°. This correlates with the devations of C16, C17 and C18 from the mean plane of the C10—C15 ring by 0.074 (6), 1.225 (6) and −0.013 (6) Å, respectively.

The dihedral angle between two benzene rings C10—C15 and C1—C6 is 16.64 (13)°. The mean plane through the enone fragment (O2/C7—C9) makes dihedral angles of 10.29 (13)° and 6.35 (14)° with C1—C6 and C10—C15 benzene ring planes, respectively.

The hydrogen bond parameters are listed in Table 1. The crystal structure is stabilized by an O—H···O hydrogen bond, leading to a C6 chain along the *c*-axis (Fig. 2). A weak C—H···π interaction also occurs (Fig. 3).

Experimental

The title compound was synthesized according to a literature method (Vogel, 1999). The compound was purified by successive recrystallization from DMF solvent. The single-crystal of (I) required for X-ray diffraction analysis was obtained by slow evaporation of a DMF solution.

Refinement

The O-bound H atom was located in a differnce map and refined as riding in its as-found relative position with U_{iso}(H) = 1.2U_{eq}(O). All the C-bound hydrogen atoms were placed in calculated positions (C—H = 0.95–0.99 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The methyl groups were allowed to rotate but not to tip to best fit the electron density.

Figures

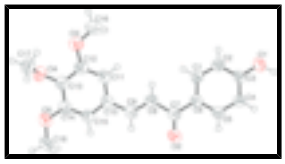

Fig. 1. View of the molecular structure of (I) showing 50% displacement ellipsoids (H atoms are drawn as spheres of arbitrary radius).

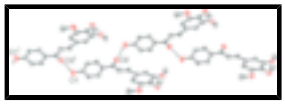

Fig. 2. Part of a C(8) chain in (I) with hydrogen bonds shown as dashed lines. All hydrogen atoms except H1 omitted for clarity. Symmetry code as in Table 1.

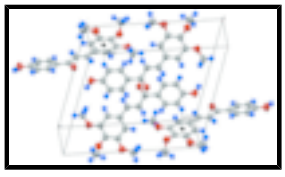

Fig. 3. The packing for (I) showing the C—H···π interaction as a dashed line.

1-(4-hydroxyphenyl)-3-(3,4,5-trimethoxyphenyl)-2-propen-1-one

Crystal data

$C_{18}H_{18}O_5$	F_{000} = 664
M_r = 314.32	D_x = 1.322 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 853 reflections
a = 12.4431 (18) Å	θ = 4.7–25.1º
b = 8.5528 (12) Å	μ = 0.10 mm^{-1}
c = 15.470 (2) Å	T = 295 (2) K
β = 106.399 (2)º	Block, pale yellow
V = 1579.4 (4) Å^3	0.25 × 0.20 × 0.20 mm
Z = 4	

Data collection

Bruker SMART1000 CCD diffractometer	3088 independent reflections
Radiation source: fine-focus sealed tube	1656 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.057
T = 295(2) K	θ_{max} = 26.0º
ω scans	θ_{min} = 4.7º
Absorption correction: multi-scan (SADABS; Bruker, 1999)	h = −15→8
T_{min} = 0.960, T_{max} = 0.981	k = −7→10
7097 measured reflections	l = −18→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.066$

$wR(F^2) = 0.179$

$S = 1.00$

3088 reflections

211 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: difmap and geom

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0929P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.33$ e Å^{-3}

$\Delta\rho_{min} = -0.20$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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}
C1	0.3208 (2)	0.4896 (3)	0.30271 (17)	0.0493 (7)
H1A	0.2754	0.4203	0.3228	0.059*
C2	0.3227 (2)	0.4838 (3)	0.21394 (17)	0.0522 (7)
H2	0.2788	0.4112	0.1747	0.063*
C3	0.3899 (2)	0.5859 (3)	0.18339 (16)	0.0480 (7)
C4	0.4558 (2)	0.6933 (4)	0.24210 (18)	0.0518 (7)
H4	0.5014	0.7618	0.2218	0.062*
C5	0.4535 (2)	0.6982 (3)	0.33056 (17)	0.0495 (7)
H5	0.4982	0.7703	0.3696	0.059*
C6	0.3858 (2)	0.5978 (3)	0.36287 (16)	0.0436 (7)
C7	0.3856 (2)	0.6078 (3)	0.45843 (17)	0.0485 (7)
C8	0.3021 (3)	0.5194 (4)	0.48890 (18)	0.0557 (8)
H8	0.2450	0.4685	0.4462	0.067*
C9	0.3050 (2)	0.5093 (4)	0.57539 (18)	0.0519 (7)
H9	0.3643	0.5603	0.6158	0.062*
C10	0.2269 (2)	0.4285 (3)	0.61475 (17)	0.0483 (7)
C11	0.1338 (2)	0.3478 (4)	0.56173 (18)	0.0540 (8)
H11	0.1209	0.3429	0.4996	0.065*
C12	0.0609 (2)	0.2754 (4)	0.60208 (19)	0.0536 (8)
C13	0.0808 (2)	0.2791 (3)	0.69571 (18)	0.0511 (7)
C14	0.1739 (2)	0.3589 (3)	0.74823 (16)	0.0487 (7)
C15	0.2463 (2)	0.4328 (3)	0.70822 (17)	0.0491 (7)
H15	0.3084	0.4857	0.7438	0.059*

C16	−0.0614 (3)	0.1908 (4)	0.4622 (2)	0.0831 (11)
H16A	−0.1310	0.1363	0.4386	0.125*
H16B	−0.0034	0.1380	0.4439	0.125*
H16C	−0.0687	0.2959	0.4395	0.125*
C17	−0.0895 (3)	0.2857 (5)	0.7318 (2)	0.0783 (10)
H17A	−0.1324	0.2294	0.7643	0.118*
H17B	−0.1326	0.2965	0.6700	0.118*
H17C	−0.0713	0.3875	0.7581	0.118*
C18	0.2756 (3)	0.4307 (5)	0.89628 (19)	0.0819 (12)
H18A	0.2731	0.4176	0.9573	0.123*
H18B	0.2713	0.5400	0.8815	0.123*
H18C	0.3444	0.3884	0.8900	0.123*
O1	0.3881 (2)	0.5740 (3)	0.09582 (12)	0.0697 (7)
H1	0.4368	0.6355	0.0742	0.084*
O2	0.45533 (17)	0.6910 (3)	0.51111 (12)	0.0603 (6)
O3	−0.03409 (19)	0.1939 (3)	0.55607 (14)	0.0720 (7)
O4	0.01136 (18)	0.2021 (3)	0.73646 (13)	0.0642 (6)
O5	0.18695 (18)	0.3539 (3)	0.83935 (12)	0.0628 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0551 (17)	0.0436 (18)	0.0499 (15)	−0.0043 (14)	0.0161 (13)	0.0026 (12)
C2	0.0619 (18)	0.0421 (18)	0.0490 (15)	−0.0073 (15)	0.0097 (14)	−0.0030 (12)
C3	0.0564 (17)	0.0438 (17)	0.0420 (14)	0.0032 (14)	0.0110 (13)	0.0038 (12)
C4	0.0531 (16)	0.0484 (19)	0.0519 (16)	−0.0040 (14)	0.0119 (13)	0.0067 (13)
C5	0.0512 (16)	0.0461 (18)	0.0467 (14)	−0.0048 (14)	0.0062 (12)	−0.0021 (12)
C6	0.0442 (14)	0.0411 (17)	0.0437 (13)	0.0049 (13)	0.0098 (12)	0.0024 (12)
C7	0.0501 (16)	0.0484 (18)	0.0469 (14)	0.0090 (14)	0.0135 (13)	−0.0009 (13)
C8	0.0549 (17)	0.061 (2)	0.0496 (16)	−0.0004 (16)	0.0114 (14)	−0.0013 (14)
C9	0.0556 (17)	0.0503 (18)	0.0491 (15)	0.0059 (15)	0.0137 (14)	−0.0006 (13)
C10	0.0548 (16)	0.0439 (18)	0.0465 (15)	0.0090 (14)	0.0146 (13)	0.0032 (12)
C11	0.0608 (17)	0.057 (2)	0.0417 (14)	0.0041 (16)	0.0107 (13)	0.0013 (13)
C12	0.0546 (17)	0.0496 (19)	0.0520 (15)	0.0019 (15)	0.0077 (13)	−0.0012 (13)
C13	0.0540 (16)	0.0469 (18)	0.0530 (16)	0.0065 (15)	0.0163 (14)	0.0063 (13)
C14	0.0571 (16)	0.0474 (18)	0.0405 (14)	0.0129 (15)	0.0120 (13)	0.0030 (12)
C15	0.0514 (16)	0.0450 (18)	0.0489 (15)	0.0022 (14)	0.0107 (13)	−0.0021 (12)
C16	0.079 (2)	0.079 (3)	0.072 (2)	−0.008 (2)	−0.0092 (18)	−0.0128 (18)
C17	0.064 (2)	0.095 (3)	0.084 (2)	0.000 (2)	0.0335 (18)	0.008 (2)
C18	0.117 (3)	0.085 (3)	0.0390 (16)	−0.009 (2)	0.0151 (18)	−0.0043 (16)
O1	0.0941 (17)	0.0699 (16)	0.0458 (11)	−0.0159 (13)	0.0208 (11)	0.0009 (9)
O2	0.0637 (13)	0.0664 (15)	0.0508 (11)	−0.0055 (11)	0.0159 (10)	−0.0122 (10)
O3	0.0737 (14)	0.0739 (17)	0.0663 (13)	−0.0146 (13)	0.0162 (11)	−0.0057 (11)
O4	0.0677 (13)	0.0592 (15)	0.0684 (13)	−0.0011 (12)	0.0236 (11)	0.0114 (10)
O5	0.0721 (14)	0.0710 (15)	0.0460 (10)	0.0003 (12)	0.0179 (10)	0.0016 (10)

Geometric parameters (Å, °)

C1—C2	1.381 (4)	C11—H11	0.9300

C1—C6	1.397 (4)	C12—O3	1.384 (3)
C1—H1A	0.9300	C12—C13	1.399 (4)
C2—C3	1.381 (4)	C13—O4	1.373 (3)
C2—H2	0.9300	C13—C14	1.392 (4)
C3—O1	1.352 (3)	C14—O5	1.373 (3)
C3—C4	1.386 (4)	C14—C15	1.382 (4)
C4—C5	1.377 (4)	C15—H15	0.9300
C4—H4	0.9300	C16—O3	1.395 (4)
C5—C6	1.391 (4)	C16—H16A	0.9600
C5—H5	0.9300	C16—H16B	0.9600
C6—C7	1.481 (4)	C16—H16C	0.9600
C7—O2	1.235 (3)	C17—O4	1.429 (4)
C7—C8	1.466 (4)	C17—H17A	0.9600
C8—C9	1.331 (4)	C17—H17B	0.9600
C8—H8	0.9300	C17—H17C	0.9600
C9—C10	1.458 (4)	C18—O5	1.369 (4)
C9—H9	0.9300	C18—H18A	0.9600
C10—C15	1.398 (3)	C18—H18B	0.9600
C10—C11	1.398 (4)	C18—H18C	0.9600
C11—C12	1.384 (4)	O1—H1	0.9331
C2—C1—C6	121.1 (3)	O3—C12—C13	114.8 (3)
C2—C1—H1A	119.5	C11—C12—C13	120.6 (3)
C6—C1—H1A	119.5	O4—C13—C14	119.7 (2)
C3—C2—C1	120.0 (3)	O4—C13—C12	120.9 (3)
C3—C2—H2	120.0	C14—C13—C12	119.4 (3)
C1—C2—H2	120.0	O5—C14—C15	124.8 (3)
O1—C3—C2	117.0 (3)	O5—C14—C13	114.9 (3)
O1—C3—C4	123.1 (3)	C15—C14—C13	120.2 (2)
C2—C3—C4	119.9 (2)	C14—C15—C10	120.5 (3)
C5—C4—C3	119.8 (3)	C14—C15—H15	119.7
C5—C4—H4	120.1	C10—C15—H15	119.7
C3—C4—H4	120.1	O3—C16—H16A	109.5
C4—C5—C6	121.5 (3)	O3—C16—H16B	109.5
C4—C5—H5	119.3	H16A—C16—H16B	109.5
C6—C5—H5	119.3	O3—C16—H16C	109.5
C5—C6—C1	117.7 (2)	H16A—C16—H16C	109.5
C5—C6—C7	119.6 (2)	H16B—C16—H16C	109.5
C1—C6—C7	122.6 (3)	O4—C17—H17A	109.5
O2—C7—C8	121.0 (2)	O4—C17—H17B	109.5
O2—C7—C6	119.6 (3)	H17A—C17—H17B	109.5
C8—C7—C6	119.5 (3)	O4—C17—H17C	109.5
C9—C8—C7	122.4 (3)	H17A—C17—H17C	109.5
C9—C8—H8	118.8	H17B—C17—H17C	109.5
C7—C8—H8	118.8	O5—C18—H18A	109.5
C8—C9—C10	128.2 (3)	O5—C18—H18B	109.5
C8—C9—H9	115.9	H18A—C18—H18B	109.5
C10—C9—H9	115.9	O5—C18—H18C	109.5
C15—C10—C11	119.5 (3)	H18A—C18—H18C	109.5
C15—C10—C9	118.6 (3)	H18B—C18—H18C	109.5

C11—C10—C9	121.9 (2)	C3—O1—H1	119.2
C12—C11—C10	119.8 (2)	C12—O3—C16	117.8 (3)
C12—C11—H11	120.1	C13—O4—C17	113.3 (2)
C10—C11—H11	120.1	C18—O5—C14	119.1 (2)
O3—C12—C11	124.5 (3)		
C6—C1—C2—C3	0.1 (4)	C10—C11—C12—O3	179.4 (3)
C1—C2—C3—O1	179.9 (3)	C10—C11—C12—C13	−1.4 (4)
C1—C2—C3—C4	0.4 (4)	O3—C12—C13—O4	1.9 (4)
O1—C3—C4—C5	−179.8 (3)	C11—C12—C13—O4	−177.3 (3)
C2—C3—C4—C5	−0.4 (4)	O3—C12—C13—C14	−179.6 (3)
C3—C4—C5—C6	−0.3 (4)	C11—C12—C13—C14	1.1 (4)
C4—C5—C6—C1	0.8 (4)	O4—C13—C14—O5	−0.7 (4)
C4—C5—C6—C7	−179.7 (3)	C12—C13—C14—O5	−179.2 (2)
C2—C1—C6—C5	−0.7 (4)	O4—C13—C14—C15	178.0 (3)
C2—C1—C6—C7	179.8 (3)	C12—C13—C14—C15	−0.5 (4)
C5—C6—C7—O2	−9.0 (4)	O5—C14—C15—C10	178.7 (2)
C1—C6—C7—O2	170.5 (3)	C13—C14—C15—C10	0.1 (4)
C5—C6—C7—C8	170.6 (3)	C11—C10—C15—C14	−0.4 (4)
C1—C6—C7—C8	−9.9 (4)	C9—C10—C15—C14	179.4 (3)
O2—C7—C8—C9	−8.0 (4)	C11—C12—O3—C16	−3.3 (4)
C6—C7—C8—C9	172.3 (3)	C13—C12—O3—C16	177.5 (3)
C7—C8—C9—C10	178.8 (3)	C14—C13—O4—C17	101.8 (3)
C8—C9—C10—C15	179.9 (3)	C12—C13—O4—C17	−79.7 (3)
C8—C9—C10—C11	−0.3 (5)	C15—C14—O5—C18	2.1 (4)
C15—C10—C11—C12	1.1 (4)	C13—C14—O5—C18	−179.3 (3)
C9—C10—C11—C12	−178.8 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.93	1.83	2.660 (3)	147
C2—H2···Cg1^{ii}	0.93	2.72	3.536 (3)	147

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

Fig. 1

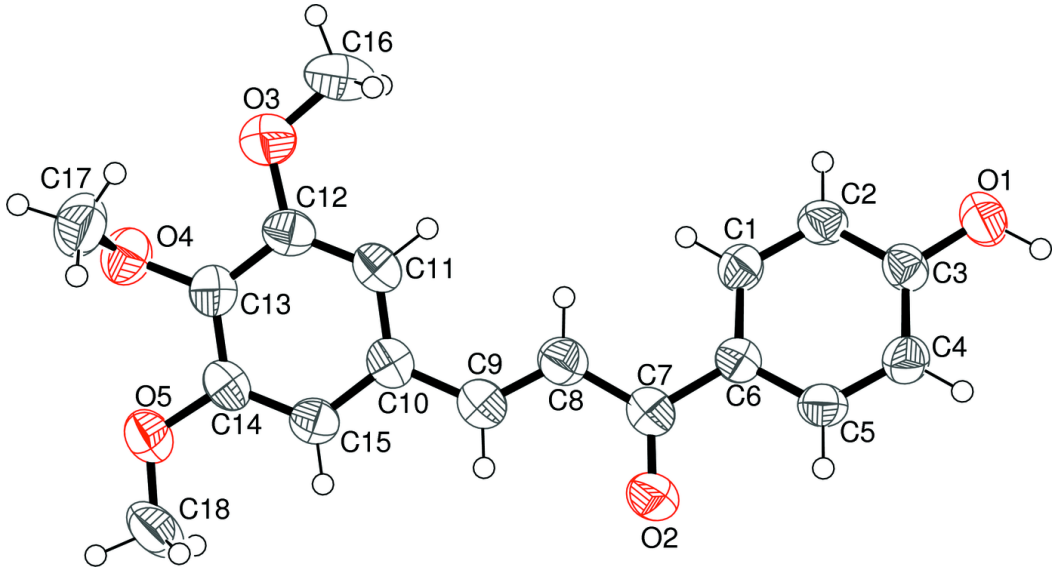
C16
O3
C17
C12
O4
C11
C13
C9
C10
O5
C14
C15
C8
C7
C6
C1
C2
O1
C3
C4
C5
C18
O2

Fig. 2

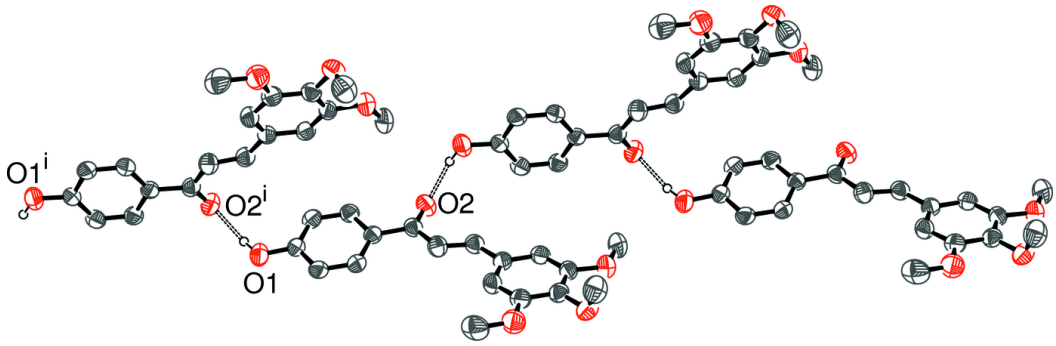

Fig. 3