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3-(4-Hydroxyphenyl)-7-(phenylsulfonyl)-4*H*-chromen-4-one

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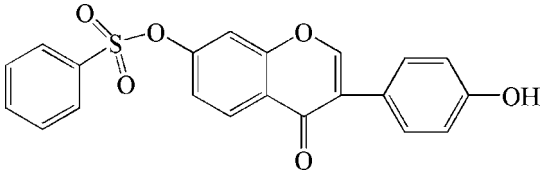
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.145; data-to-parameter ratio = 17.1.

The title compound, $C_{21}H_{14}O_6S$, is a new daidzein derivative with potential medical applications. The hydroxyphenyl ring makes a dihedral angle of 51.31 (8)° with the benzopyranone ring. The crystal structure is stabilized by intermolecular O—H···O and C—H···O hydrogen bonds.

Related literature

For general background, see: Tlkkanen *et al.* (1998); Sarhyyamoonhy & Wang (1997). For related structures, see: Wang & Zhang (2005); Zhang, Wang, He & Yu (2005); Zhang, Wang, Wang & Wu (2005).



Experimental

Crystal data

$C_{21}H_{14}O_6S$
M_r = 394.37
Monoclinic, $P2_1/n$
a = 6.1408 (3) Å
b = 13.0272 (7) Å
c = 22.7381 (12) Å
β = 91.891 (1)°
V = 1818.00 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 293 (2) K
0.35 × 0.26 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.868, T_{max} = 0.970
13556 measured reflections
4314 independent reflections
2478 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.145
S = 1.07
4314 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6A···O5^{i}	0.82	1.91	2.716 (2)	170
C7—H7A···O1^{ii}	0.93	2.59	3.216 (5)	125
C12—H12A···O1^{iii}	0.93	2.45	3.139 (5)	131
C14—H14A···O4^{ii}	0.93	2.47	3.345 (5)	156
C17—H17A···O2^{iv}	0.93	2.52	3.234 (5)	134

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); 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: XU2361).

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supplementary materials

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3-(4-Hydroxyphenyl)-7-(phenylsulfonyl)-4*H*-chromen-4-one

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Comment

Daidzein and its derivatives have obtained much attention for their potential antidysrhythmic, antioxidant, effective in getting rid of hyperkinesias (Tlkkanen, 1998) and in inhibiting cancer cells growth (Sarhyyamoonhy & Wang, 1997). The title compound is a novel daidzein derivative with potential medical applications, its crystal structure is reported here.

The title compound is composed with a benzopyranone, a benzensulfonate and a hydroxyl group (Figure 1). The atoms of benzopyranone moiety (C7—C15, O4) is almost coplanar with a mean deviation 0.028 Å form the least square plane. To avoid steric conflicts, hydroxyphenyl ring (C1—C6) and benzopyranone moiety are twisted by 51.31 (8)°. The crystal structure is stabilized by intermolecular O—H···O and C—H···O hydrogen bonds (Table 1 and Figure 2).

Experimental

A solution of daidzein (101 mg, 0.4 mmol) and t-BuONa (10 mg) in dry CH_2Cl_2 (15 ml) is stirred at −20 °C for 2.5 h under Ar atmosphere. Then the benzene sulfonic acid chloride (68 mg, 0.48 mmol) in CH_2Cl_2 (2 ml) is instilled in 20 minutes and the reacts for a further 0.5 h. Pouring into ice water followed by extraction with ether/ethyl acetate (1/2), washing with aqueous solution of $NaHCO_3$, drying and removal of solvent under reduced pressure give the crude product. Purification by flash chromatography (silica, $CHCl_3$/$(CH_3)_2CO$, 10/1, V/V) yields the title compound (Yield: 80%). Single crystals were grown by slow evaporation from a CH_2Cl_2/$(CH_3)_2CO$ (1:1 *v*/*v*) solution.

Refinement

All H atoms were positioned geometrically with O—H = 0.82 and C—H = 0.93 Å and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O).

Figures

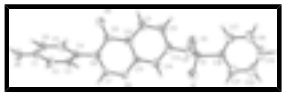

Fig. 1. Perspective structure of compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

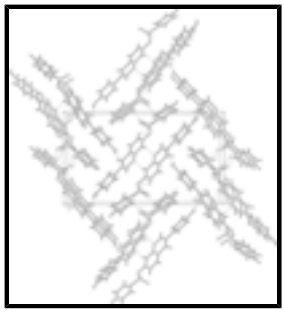

Fig. 2. The packing of (I), view down the *a* axis.

3-(4-Hydroxyphenyl)-7-(phenylsulfonyl)-4*H*-chromen-4-one

Crystal data

$C_{21}H_{14}O_6S$	F_{000} = 816
M_r = 394.37	D_x = 1.441 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 268-270 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 6.1408 (3) Å	θ = 2.7–24.2º
b = 13.0272 (7) Å	μ = 0.22 mm^{-1}
c = 22.7381 (12) Å	T = 293 (2) K
β = 91.891 (1)º	Block, yellow
V = 1818.00 (16) Å^3	0.35 × 0.26 × 0.14 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	4314 independent reflections
Radiation source: fine-focus sealed tube	2478 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.037
T = 293(2) K	θ_{max} = 28.4º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −7→8
T_{min} = 0.868, T_{max} = 0.970	k = −17→17
13556 measured reflections	l = −30→30

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H-atom parameters constrained
$wR(F^2)$ = 0.145	$w = 1/[\sigma^2(F_o^2) + (0.0558P)^2 + 0.1514P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.002
4314 reflections	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
253 parameters	$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 $F^2 > 2\text{sigma}(F^2)$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.0869 (4)	−0.33515 (15)	0.72589 (9)	0.0568 (5)
C2	0.2690 (4)	−0.27307 (17)	0.73315 (10)	0.0663 (6)
H2B	0.3878	−0.2821	0.7093	0.080*
C3	0.2735 (4)	−0.19784 (16)	0.77581 (9)	0.0609 (5)
H3A	0.3967	−0.1568	0.7806	0.073*
C4	0.0992 (3)	−0.18196 (14)	0.81162 (8)	0.0505 (5)
C5	−0.0829 (4)	−0.24414 (15)	0.80349 (9)	0.0576 (5)
H5A	−0.2026	−0.2345	0.8269	0.069*
C6	−0.0885 (4)	−0.32037 (15)	0.76103 (9)	0.0585 (5)
H6B	−0.2113	−0.3617	0.7562	0.070*
C7	0.2899 (4)	−0.09870 (16)	0.89349 (10)	0.0662 (6)
H7A	0.3915	−0.1509	0.8892	0.079*
C8	0.1129 (3)	−0.10184 (14)	0.85800 (8)	0.0516 (5)
C9	−0.0542 (4)	−0.02307 (15)	0.86390 (8)	0.0540 (5)
C10	−0.0039 (4)	0.05562 (15)	0.90851 (8)	0.0549 (5)
C11	−0.1410 (4)	0.13926 (17)	0.91859 (11)	0.0706 (6)
H11A	−0.2717	0.1451	0.8970	0.085*
C12	−0.0862 (4)	0.21275 (19)	0.95980 (10)	0.0751 (7)
H12A	−0.1767	0.2689	0.9654	0.090*
C13	0.1040 (4)	0.20204 (16)	0.99268 (9)	0.0639 (6)
C14	0.2446 (4)	0.12272 (16)	0.98480 (9)	0.0680 (6)
H14A	0.3737	0.1171	1.0071	0.082*
C15	0.1870 (4)	0.05051 (15)	0.94200 (9)	0.0587 (5)
C16	0.3035 (4)	0.43441 (15)	1.08865 (9)	0.0612 (6)
C17	0.1139 (5)	0.48937 (19)	1.09136 (11)	0.0829 (8)
H17A	0.0034	0.4812	1.0628	0.099*
C18	0.0902 (6)	0.5571 (2)	1.13742 (13)	0.1043 (10)
H18A	−0.0386	0.5941	1.1402	0.125*
C19	0.2521 (8)	0.5704 (2)	1.17862 (14)	0.1068 (11)
H19A	0.2352	0.6175	1.2088	0.128*
C20	0.4413 (6)	0.5145 (3)	1.17591 (12)	0.1038 (10)
H20A	0.5511	0.5233	1.2046	0.125*
C21	0.4693 (5)	0.4449 (2)	1.13051 (11)	0.0803 (7)

H21A	0.5965	0.4064	1.1284	0.096*
O1	0.5432 (3)	0.30065 (15)	1.03724 (8)	0.0927 (6)
O2	0.3030 (3)	0.40496 (13)	0.97484 (7)	0.0860 (5)
O3	0.1485 (3)	0.27485 (12)	1.03782 (6)	0.0761 (5)
O4	0.3361 (3)	−0.02712 (11)	0.93507 (7)	0.0760 (5)
O5	−0.2233 (3)	−0.02273 (12)	0.83326 (7)	0.0742 (5)
O6	0.0906 (3)	−0.40877 (12)	0.68330 (7)	0.0800 (5)
H6A	−0.0266	−0.4389	0.6817	0.120*
S1	0.34440 (10)	0.35395 (4)	1.02870 (2)	0.0632 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0578 (13)	0.0487 (10)	0.0637 (12)	−0.0001 (9)	0.0000 (10)	−0.0077 (9)
C2	0.0549 (14)	0.0698 (14)	0.0748 (14)	−0.0054 (11)	0.0117 (11)	−0.0147 (12)
C3	0.0559 (13)	0.0570 (12)	0.0699 (13)	−0.0089 (10)	0.0015 (10)	−0.0078 (10)
C4	0.0579 (13)	0.0434 (10)	0.0501 (10)	−0.0001 (9)	−0.0005 (9)	0.0028 (8)
C5	0.0591 (14)	0.0552 (11)	0.0589 (12)	−0.0020 (10)	0.0095 (10)	0.0012 (9)
C6	0.0547 (13)	0.0509 (11)	0.0702 (13)	−0.0073 (9)	0.0039 (10)	−0.0004 (10)
C7	0.0804 (17)	0.0491 (11)	0.0679 (13)	0.0139 (11)	−0.0152 (12)	−0.0079 (10)
C8	0.0617 (13)	0.0455 (10)	0.0474 (10)	0.0012 (9)	−0.0001 (9)	0.0054 (8)
C9	0.0606 (14)	0.0519 (11)	0.0495 (10)	0.0016 (10)	0.0025 (10)	0.0004 (9)
C10	0.0615 (13)	0.0539 (11)	0.0497 (10)	0.0026 (9)	0.0091 (9)	0.0004 (9)
C11	0.0595 (14)	0.0739 (14)	0.0784 (15)	0.0075 (11)	0.0050 (11)	−0.0190 (12)
C12	0.0702 (17)	0.0722 (15)	0.0838 (16)	0.0087 (12)	0.0178 (13)	−0.0202 (13)
C13	0.0827 (17)	0.0595 (13)	0.0502 (11)	−0.0064 (11)	0.0138 (11)	−0.0107 (10)
C14	0.0893 (17)	0.0593 (13)	0.0546 (12)	0.0023 (12)	−0.0097 (11)	−0.0062 (10)
C15	0.0755 (15)	0.0515 (11)	0.0490 (11)	0.0092 (10)	−0.0014 (10)	−0.0005 (9)
C16	0.0792 (16)	0.0512 (11)	0.0532 (11)	−0.0038 (11)	0.0051 (11)	−0.0004 (9)
C17	0.111 (2)	0.0705 (15)	0.0670 (15)	0.0240 (15)	0.0001 (14)	−0.0083 (12)
C18	0.148 (3)	0.0760 (18)	0.091 (2)	0.0253 (19)	0.025 (2)	−0.0175 (16)
C19	0.165 (4)	0.0735 (18)	0.083 (2)	−0.024 (2)	0.031 (2)	−0.0283 (16)
C20	0.126 (3)	0.113 (2)	0.0724 (18)	−0.049 (2)	0.0073 (17)	−0.0213 (17)
C21	0.0835 (19)	0.0839 (17)	0.0735 (15)	−0.0187 (14)	0.0048 (13)	−0.0070 (13)
O1	0.0817 (13)	0.0918 (12)	0.1048 (14)	0.0246 (10)	0.0074 (10)	−0.0163 (10)
O2	0.1241 (15)	0.0812 (11)	0.0531 (9)	−0.0028 (10)	0.0081 (9)	0.0042 (8)
O3	0.0980 (13)	0.0692 (9)	0.0625 (9)	−0.0163 (9)	0.0243 (8)	−0.0227 (8)
O4	0.0939 (12)	0.0599 (9)	0.0718 (10)	0.0223 (8)	−0.0319 (9)	−0.0154 (8)
O5	0.0672 (11)	0.0733 (10)	0.0809 (10)	0.0155 (8)	−0.0145 (9)	−0.0142 (8)
O6	0.0708 (11)	0.0750 (10)	0.0951 (12)	−0.0122 (8)	0.0124 (9)	−0.0362 (9)
S1	0.0747 (4)	0.0586 (3)	0.0570 (3)	0.0038 (3)	0.0117 (3)	−0.0044 (2)

Geometric parameters (Å, °)

C1—O6	1.364 (2)	C12—H12A	0.9300
C1—C6	1.376 (3)	C13—C14	1.362 (3)
C1—C2	1.386 (3)	C13—O3	1.417 (2)
C2—C3	1.379 (3)	C14—C15	1.391 (3)
C2—H2B	0.9300	C14—H14A	0.9300

C3—C4	1.382 (3)	C15—O4	1.377 (2)
C3—H3A	0.9300	C16—C17	1.370 (3)
C4—C5	1.388 (3)	C16—C21	1.378 (3)
C4—C8	1.484 (3)	C16—S1	1.744 (2)
C5—C6	1.385 (3)	C17—C18	1.381 (3)
C5—H5A	0.9300	C17—H17A	0.9300
C6—H6B	0.9300	C18—C19	1.354 (5)
C7—C8	1.333 (3)	C18—H18A	0.9300
C7—O4	1.351 (2)	C19—C20	1.374 (5)
C7—H7A	0.9300	C19—H19A	0.9300
C8—C9	1.461 (3)	C20—C21	1.389 (4)
C9—O5	1.231 (2)	C20—H20A	0.9300
C9—C10	1.468 (3)	C21—H21A	0.9300
C10—C15	1.378 (3)	O1—S1	1.4122 (18)
C10—C11	1.401 (3)	O2—S1	1.4091 (17)
C11—C12	1.374 (3)	O3—S1	1.6027 (17)
C11—H11A	0.9300	O6—H6A	0.8200
C12—C13	1.373 (3)		
O6—C1—C6	122.86 (19)	C14—C13—C12	122.5 (2)
O6—C1—C2	117.57 (19)	C14—C13—O3	119.7 (2)
C6—C1—C2	119.56 (19)	C12—C13—O3	117.8 (2)
C3—C2—C1	119.7 (2)	C13—C14—C15	117.2 (2)
C3—C2—H2B	120.1	C13—C14—H14A	121.4
C1—C2—H2B	120.1	C15—C14—H14A	121.4
C2—C3—C4	121.6 (2)	O4—C15—C10	121.94 (18)
C2—C3—H3A	119.2	O4—C15—C14	115.0 (2)
C4—C3—H3A	119.2	C10—C15—C14	123.1 (2)
C3—C4—C5	118.05 (18)	C17—C16—C21	121.8 (2)
C3—C4—C8	119.81 (18)	C17—C16—S1	119.59 (18)
C5—C4—C8	122.12 (18)	C21—C16—S1	118.51 (19)
C6—C5—C4	120.86 (19)	C16—C17—C18	118.6 (3)
C6—C5—H5A	119.6	C16—C17—H17A	120.7
C4—C5—H5A	119.6	C18—C17—H17A	120.7
C1—C6—C5	120.22 (19)	C19—C18—C17	120.8 (3)
C1—C6—H6B	119.9	C19—C18—H18A	119.6
C5—C6—H6B	119.9	C17—C18—H18A	119.6
C8—C7—O4	126.4 (2)	C18—C19—C20	120.2 (3)
C8—C7—H7A	116.8	C18—C19—H19A	119.9
O4—C7—H7A	116.8	C20—C19—H19A	119.9
C7—C8—C9	118.96 (18)	C19—C20—C21	120.3 (3)
C7—C8—C4	118.55 (18)	C19—C20—H20A	119.8
C9—C8—C4	122.39 (18)	C21—C20—H20A	119.8
O5—C9—C8	122.18 (18)	C16—C21—C20	118.1 (3)
O5—C9—C10	122.89 (19)	C16—C21—H21A	120.9
C8—C9—C10	114.93 (18)	C20—C21—H21A	120.9
C15—C10—C11	116.89 (19)	C13—O3—S1	117.65 (13)
C15—C10—C9	120.26 (18)	C7—O4—C15	117.50 (17)
C11—C10—C9	122.8 (2)	C1—O6—H6A	109.5
C12—C11—C10	121.2 (2)	O2—S1—O1	118.79 (12)

C12—C11—H11A	119.4	O2—S1—O3	107.52 (11)
C10—C11—H11A	119.4	O1—S1—O3	108.38 (11)
C13—C12—C11	119.0 (2)	O2—S1—C16	111.67 (10)
C13—C12—H12A	120.5	O1—S1—C16	109.52 (11)
C11—C12—H12A	120.5	O3—S1—C16	99.05 (9)
O6—C1—C2—C3	−179.7 (2)	O3—C13—C14—C15	176.60 (18)
C6—C1—C2—C3	0.6 (3)	C11—C10—C15—O4	−178.69 (19)
C1—C2—C3—C4	−0.4 (3)	C9—C10—C15—O4	0.1 (3)
C2—C3—C4—C5	−0.1 (3)	C11—C10—C15—C14	0.9 (3)
C2—C3—C4—C8	178.48 (19)	C9—C10—C15—C14	179.78 (19)
C3—C4—C5—C6	0.5 (3)	C13—C14—C15—O4	179.0 (2)
C8—C4—C5—C6	−178.03 (18)	C13—C14—C15—C10	−0.7 (3)
O6—C1—C6—C5	−179.87 (19)	C21—C16—C17—C18	0.2 (4)
C2—C1—C6—C5	−0.2 (3)	S1—C16—C17—C18	−176.3 (2)
C4—C5—C6—C1	−0.4 (3)	C16—C17—C18—C19	1.1 (4)
O4—C7—C8—C9	−1.5 (3)	C17—C18—C19—C20	−1.6 (5)
O4—C7—C8—C4	175.1 (2)	C18—C19—C20—C21	0.9 (5)
C3—C4—C8—C7	−48.2 (3)	C17—C16—C21—C20	−0.9 (4)
C5—C4—C8—C7	130.3 (2)	S1—C16—C21—C20	175.61 (18)
C3—C4—C8—C9	128.2 (2)	C19—C20—C21—C16	0.3 (4)
C5—C4—C8—C9	−53.2 (3)	C14—C13—O3—S1	71.8 (2)
C7—C8—C9—O5	−178.6 (2)	C12—C13—O3—S1	−110.7 (2)
C4—C8—C9—O5	5.0 (3)	C8—C7—O4—C15	0.1 (3)
C7—C8—C9—C10	2.0 (3)	C10—C15—O4—C7	0.6 (3)
C4—C8—C9—C10	−174.41 (17)	C14—C15—O4—C7	−179.11 (19)
O5—C9—C10—C15	179.2 (2)	C13—O3—S1—O2	55.51 (18)
C8—C9—C10—C15	−1.4 (3)	C13—O3—S1—O1	−74.07 (18)
O5—C9—C10—C11	−2.0 (3)	C13—O3—S1—C16	171.77 (17)
C8—C9—C10—C11	177.38 (19)	C17—C16—S1—O2	50.1 (2)
C15—C10—C11—C12	0.3 (3)	C21—C16—S1—O2	−126.49 (19)
C9—C10—C11—C12	−178.5 (2)	C17—C16—S1—O1	−176.26 (19)
C10—C11—C12—C13	−1.8 (4)	C21—C16—S1—O1	7.2 (2)
C11—C12—C13—C14	2.1 (4)	C17—C16—S1—O3	−63.0 (2)
C11—C12—C13—O3	−175.4 (2)	C21—C16—S1—O3	120.47 (19)
C12—C13—C14—C15	−0.8 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6A···O5^{i}	0.82	1.91	2.716 (2)	170
C7—H7A···O1^{ii}	0.93	2.59	3.216 (5)	125
C12—H12A···O1^{iii}	0.93	2.45	3.139 (5)	131
C14—H14A···O4^{ii}	0.93	2.47	3.345 (5)	156
C17—H17A···O2^{iv}	0.93	2.52	3.234 (5)	134

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

Fig. 1

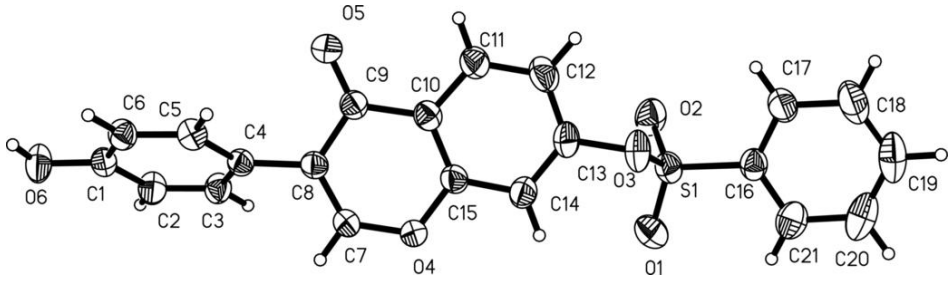
O5
C11
C9
C10
C12
C17
C6
C5
C4
O2
C18
O6
C1
C2
C3
C8
C15
C14
C13
O3
S1
C16
C19
C7
O4
O1
C21
C20

Fig. 2