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5-(2-Benzoylethenyl)-*N*-benzyl-2-methoxybenzenesulfonamide

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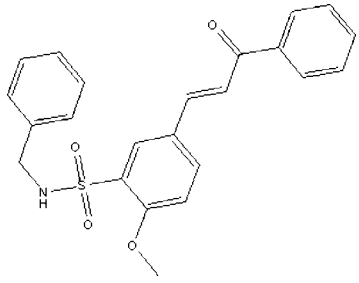
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.135; data-to-parameter ratio = 13.1.

Singly, sulfonamide and chalcone are well known pharmacophoric groups which have several pharmaceutical applications for a variety of diseases. Combination of two or more pharmacophoric groups can enhance the probability of discovering new lead compounds, especially if closely related activities are involved. The title compound, $C_{23}H_{21}NO_4S$, was prepared in order to investigate its potential clinical application. It shows an interesting molecule that shows a V-shaped molecular structure formed by sulfonamide and chalcone arms. The chalcone group is quasi-planar and the sulfonamide aromatic ring is almost perpendicular to the mean plane of the chalcone. An infinite zigzag chain parallel to the crystallographic axis [001] results from intermolecular N—H···O hydrogen bonds and keeps the molecules perfectly stacked in this direction.

Related literature

For related literature, see: Bhattacharya *et al.* (2004); Cremlyn *et al.* (1984); Dominguez *et al.* (2005); Lunardi *et al.* (2003); Ni *et al.* (2004); Subbiah Pandi *et al.* (2003); Petersen (2004); Rojas *et al.* (2002); Supuran *et al.* (2003).



Experimental

Crystal data

$C_{23}H_{21}NO_4S$
M_r = 407.47
Triclinic, $P\overline{1}$
a = 10.3671 (12) Å
b = 10.3750 (8) Å
c = 10.7977 (14) Å
α = 84.88 (1)°
β = 68.79 (1)°
γ = 65.40 (1)°
V = 981.9 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 293 (2) K
0.50 × 0.33 × 0.13 mm

Data collection

Enraf-Nonius CAD-4 diffractometer
Absorption correction: ψ scan (*PLATON*; Spek, 2003; North *et al.*, 1968)
T_{min} = 0.924, T_{max} = 0.969
3694 measured reflections
3490 independent reflections
2573 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
3 standard reflections
every 200 reflections
intensity decay: <1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.135
S = 1.05
3490 reflections
266 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O171^{i}	0.84 (3)	2.23 (3)	3.018 (3)	156 (3)

Symmetry code: (i) $x, y, z-1$.

Data collection: *CAD-4 EXPRESS* (Enraf-Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *HELENA* (Spek, 1996); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97* and *MOGUL* (Bruno *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2110).

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supplementary materials

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5-(2-Benzoylethenyl)-*N*-benzyl-2-methoxybenzenesulfonamide

C. R. Andrighetti-Fröhner, A. C. Joussef, C. M. O. Simões, R. J. Nunes and A. J. Bortoluzzi

Comment

Sulfonamide is a pharmacophoric group of over than 30 pharmaceuticals which are in clinical use, with antibacterial, diuretic, oral antidiabetic, HIV protease inhibitory (Supuran *et al.*, 2003) and antimalarial (Petersen, 2004) activities. Many novel sulfonamide derivatives have recently been reported to show carbonic anhydrase inhibitory action, matrix metalloproteinase inhibitory action, endothelin receptor antagonism, antitumoral (Supuran *et al.*, 2003) and antileishmanial (Bhattacharya *et al.*, 2004) activities.

Naturally occurring and synthetic chalcones are known to have a wide range of potential pharmacological activities, such as anti-inflammatory, antibacterial, anticancer, antiviral, antimalarial (Ni *et al.*, 2004), antitrypanosomal, antileishmanial (Lunardi *et al.*, 2003) and nitric oxide inhibitory action (Rojas *et al.*, 2002). A combination of two or more pharmacophoric groups can enhance the discovery probability of new lead compounds, specially if closely related activities are involved. Recently, analogs of sulfonamide chalcone derivatives were synthesized and showed activity against cultured *Plasmodium falciparum* parasites (Dominguez *et al.*, 2005). In order to investigate of bioactivity of the combined compounds, we have prepared some sulfonamide chalcone derivatives, and in this paper we present the synthesis and X-ray study of (I).

The molecule of (I) shows an angular geometry (Fig. 1) resulting from the structural combination of sulfonamide and chalcone moieties, with the vertices of the molecule occupied by S atom. The chalcone arm is quasi planar, where the dihedral angles between the best planes of the rings C9···C14 and C18···C23 is 10.85 (6)° and the best plane of the central chain C13—C15═C16—C17 with respect to phenyl rings C9···C14 and C18···C23 are 10.4 (1)° and 11.6 (1)°, respectively. This feature suggests that there is electronic delocalization forming an extended π -electron conjugated system in this moiety. It is in accord with decreased length of the C16—C17 [1.471 (3) Å] single bond and the increased length of the C15═C16 [1.322 (4) Å] double bond. In addition, the methoxy group is also almost coplanar with its attached phenyl ring. It was observed in similar structures of chalcone (Subbiah Pandi *et al.*, 2003 and cited references) when the mehtoxy is in *para* position with respect to the central chain. In the sulfonamide moiety, the distances and angles around N1 and C2 are within the expected range found in similar structures searched in CSD V5.28 with Mogul (Bruno *et al.*, 2004). The phenyl ring C3···C8 is almost perpendicular to the mean plane of the chalcone arm, where the dihedral angle between these planes is 85.04 (8)°. An intermolecular hydrogen bond [N1—H1···O171^{i}, NH = 0.84 (3) Å, H···O = 2.23 (3) Å, N—H···O = 156 (3)°, symmetry code: (i) $x, y, z-1$] promotes a zigzag infinite chain formation running parallel to the crystallographic [001] axis (Fig. 2), keeping the molecules stacked in this direction.

Experimental

Compound (I) was synthesized according to the method of Cremlyn *et al.* (1984). 4-methoxychalcone (6.63 g, 27.87 mmol), was reacted with chlorosulphonic acid (19.48 g, 167.2 mmol) at room temperature for 1 week. The red solution was poured onto crushed ice with stirring to give the sulfonyl chloride as a yellow solid. The sulfonyl chloride (0.50 g, 1.48 mmol) was treated with benzylamine (0.23 g, 2.19 mmol) in methanol at 273 K. The mixture was reacted at room temperature for 1 h and was then poured onto ice-water. The precipitate was collected by filtration, washed with cold methanol, dried

and recrystallized in hot ethanol (yield 0.25 g, 42%). *M*.p. 167–170°C (yellow crystalline solid). Colourless single crystals suitable for X-ray analysis were obtained by slow evaporation of a chloroform solution. ^{1}H NMR ($CDCl_3$): δ: 3.89 (s, 3H, OCH_3), 4.17 (d, *J*=6.19 Hz, 2H, CH_2), 6.92–8.28 (m, 13H, ArH, 2H olefinic H). Elemental Analysis calculated for $C_{23}H_{21}NO_4S$: C 67.79, H 5.19, N 3.44, S 7.87%; Found: C 67.52, H 5.11, N 3.50, S 7.62%.

Refinement

All non-H atoms were refined with anisotropic displacement parameters. H atoms attached to C atoms were added at their calculated positions and included in the refinement, with constrained distances C—H = 0.96 (CH_3), 0.97 (CH_2) or 0.93Å (CH_{Ar}), and U_{iso}(H) = 1.2U_{eq}(carrier C) or 1.5U_{eq}(C102) for the methyl group. Atom H1 bonded to N1 was found in a difference map and treated as an isotropic free atom.

Figures

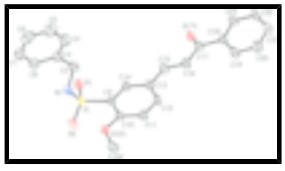

Fig. 1. The molecular structure of (I) with labeling scheme. Displacement ellipsoids are shown at the 40% probability level.

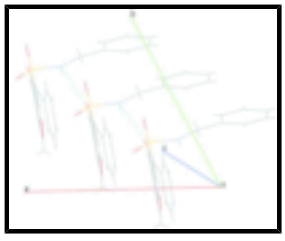

Fig. 2. Packing of (I) showing the molecules connected through hydrogen bonds and stacked along [001].

5-(2-Benzoylethenyl)-*N*-benzyl-2-methoxybenzenesulfonamide

Crystal data

$C_{23}H_{21}NO_4S$	F_{000} = 428
M_r = 407.47	D_x = 1.379 Mg m^{-3}
Triclinic, $P\overline{1}$	Melting point: 440-443 K
a = 10.3671 (12) Å	Mo *K*α radiation λ = 0.71073 Å
b = 10.3750 (8) Å	Cell parameters from 25 reflections
c = 10.7977 (14) Å	θ = 6.7–15.4º
α = 84.88 (1)º	μ = 0.20 mm^{-1}
β = 68.79 (1)º	*T* = 293 (2) K
γ = 65.40 (1)º	Irregular block, colourless
V = 981.9 (2) Å^3	0.50 × 0.33 × 0.13 mm
Z = 2	

Data collection

Enraf-Nonius CAD-4 diffractometer	R_{int} = 0.027
Radiation source: fine-focus sealed tube	θ_{max} = 25.1º
Monochromator: graphite	θ_{min} = 2.0º
T = 293(2) K	h = −12→11
ω–2θ scans	k = −12→12
Absorption correction: ψ scan (PLATON; Spek, 2003; North *et al.*, 1968)	l = −12→0
T_{min} = 0.924, T_{max} = 0.969	3 standard reflections
3694 measured reflections	every 200 reflections
3490 independent reflections	intensity decay: <1%
2573 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.135	$w = 1/[\sigma^2(F_o^2) + (0.067P)^2 + 0.4657P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
3490 reflections	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
266 parameters	$\Delta\rho_{min}$ = −0.46 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	y	z	U_{iso}*/U_{eq}
S1	0.28300 (8)	0.31669 (7)	0.78462 (6)	0.0353 (2)
O1	0.2332 (2)	0.43617 (19)	0.87332 (18)	0.0461 (5)
O2	0.4138 (2)	0.2877 (2)	0.66670 (18)	0.0484 (5)
N1	0.1427 (3)	0.3383 (2)	0.7393 (2)	0.0367 (5)
H1	0.170 (3)	0.275 (3)	0.681 (3)	0.044 (8)*
C2	−0.0055 (3)	0.3700 (3)	0.8446 (3)	0.0480 (7)
H2A	−0.0265	0.4446	0.9066	0.058*
H2B	−0.0014	0.2859	0.8932	0.058*
C3	−0.1333 (3)	0.4163 (3)	0.7925 (3)	0.0420 (7)
C4	−0.2592 (4)	0.3912 (4)	0.8631 (3)	0.0589 (9)
H4	−0.2633	0.3450	0.9414	0.071*
C5	−0.3807 (4)	0.4334 (4)	0.8197 (4)	0.0693 (10)
H5	−0.4656	0.4162	0.8689	0.083*
C6	−0.3745 (4)	0.5010 (4)	0.7030 (4)	0.0654 (10)

H6	−0.4545	0.5281	0.6723	0.079*
C7	−0.2501 (4)	0.5281 (3)	0.6327 (3)	0.0604 (9)
H7	−0.2466	0.5752	0.5549	0.073*
C8	−0.1298 (4)	0.4863 (3)	0.6762 (3)	0.0489 (7)
H8	−0.0458	0.5050	0.6273	0.059*
C9	0.3096 (3)	0.1678 (3)	0.8821 (2)	0.0315 (6)
C10	0.3649 (3)	0.0305 (3)	0.8251 (2)	0.0325 (6)
C11	0.3815 (3)	−0.0826 (3)	0.9063 (3)	0.0380 (6)
H11	0.4192	−0.1747	0.8698	0.046*
C12	0.3421 (3)	−0.0579 (3)	1.0408 (3)	0.0381 (6)
H12	0.3534	−0.1347	1.0939	0.046*
C13	0.2860 (3)	0.0776 (3)	1.1006 (2)	0.0345 (6)
C14	0.2715 (3)	0.1896 (3)	1.0186 (2)	0.0331 (6)
H14	0.2355	0.2812	1.0555	0.040*
C15	0.2394 (3)	0.1059 (3)	1.2440 (2)	0.0376 (6)
H15	0.2134	0.1980	1.2734	0.045*
C16	0.2302 (3)	0.0138 (3)	1.3362 (2)	0.0393 (6)
H16	0.2576	−0.0800	1.3102	0.047*
C17	0.1780 (3)	0.0552 (3)	1.4786 (2)	0.0362 (6)
C18	0.1533 (3)	−0.0500 (3)	1.5782 (2)	0.0348 (6)
C19	0.2058 (4)	−0.1925 (3)	1.5438 (3)	0.0468 (7)
H19	0.2517	−0.2255	1.4545	0.056*
C20	0.1905 (4)	−0.2867 (3)	1.6415 (3)	0.0562 (9)
H20	0.2259	−0.3828	1.6177	0.067*
C21	0.1231 (4)	−0.2384 (3)	1.7735 (3)	0.0519 (8)
H21	0.1144	−0.3020	1.8391	0.062*
C22	0.0689 (3)	−0.0973 (3)	1.8085 (3)	0.0477 (7)
H22	0.0222	−0.0648	1.8980	0.057*
C23	0.0829 (3)	−0.0028 (3)	1.7121 (3)	0.0407 (6)
H23	0.0449	0.0934	1.7367	0.049*
C102	0.4726 (3)	−0.1232 (3)	0.6292 (3)	0.0449 (7)
H10A	0.4882	−0.1177	0.5360	0.067*
H10B	0.4116	−0.1753	0.6687	0.067*
H10C	0.5691	−0.1708	0.6402	0.067*
O101	0.3966 (2)	0.01728 (18)	0.69291 (16)	0.0388 (5)
O171	0.1559 (3)	0.1728 (2)	1.51546 (18)	0.0480 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0476 (4)	0.0353 (4)	0.0232 (3)	−0.0175 (3)	−0.0134 (3)	0.0062 (2)
O1	0.0728 (14)	0.0373 (10)	0.0336 (10)	−0.0245 (10)	−0.0239 (10)	0.0065 (8)
O2	0.0534 (13)	0.0578 (12)	0.0324 (11)	−0.0282 (10)	−0.0082 (9)	0.0077 (9)
N1	0.0428 (13)	0.0399 (12)	0.0222 (11)	−0.0095 (10)	−0.0143 (10)	0.0004 (9)
C2	0.0459 (17)	0.0610 (19)	0.0276 (14)	−0.0138 (14)	−0.0123 (13)	0.0011 (13)
C3	0.0463 (17)	0.0397 (15)	0.0357 (15)	−0.0113 (13)	−0.0170 (13)	−0.0008 (12)
C4	0.062 (2)	0.065 (2)	0.052 (2)	−0.0281 (18)	−0.0229 (17)	0.0136 (16)
C5	0.054 (2)	0.068 (2)	0.089 (3)	−0.0280 (18)	−0.026 (2)	0.008 (2)

C6	0.062 (2)	0.058 (2)	0.079 (3)	−0.0098 (17)	−0.044 (2)	−0.0065 (18)
C7	0.064 (2)	0.058 (2)	0.054 (2)	−0.0100 (17)	−0.0330 (18)	0.0060 (15)
C8	0.0480 (18)	0.0538 (18)	0.0383 (16)	−0.0127 (14)	−0.0186 (14)	0.0050 (13)
C9	0.0362 (14)	0.0368 (13)	0.0234 (12)	−0.0145 (11)	−0.0143 (11)	0.0066 (10)
C10	0.0336 (14)	0.0394 (14)	0.0244 (13)	−0.0138 (11)	−0.0120 (11)	0.0036 (10)
C11	0.0499 (17)	0.0345 (14)	0.0293 (14)	−0.0155 (12)	−0.0166 (12)	0.0043 (11)
C12	0.0494 (16)	0.0380 (14)	0.0289 (14)	−0.0186 (13)	−0.0179 (12)	0.0115 (11)
C13	0.0379 (15)	0.0429 (14)	0.0255 (13)	−0.0189 (12)	−0.0130 (11)	0.0072 (11)
C14	0.0394 (15)	0.0345 (13)	0.0252 (13)	−0.0138 (11)	−0.0133 (11)	0.0026 (10)
C15	0.0459 (16)	0.0452 (15)	0.0260 (13)	−0.0200 (13)	−0.0167 (12)	0.0047 (11)
C16	0.0535 (17)	0.0423 (15)	0.0241 (13)	−0.0208 (13)	−0.0157 (12)	0.0054 (11)
C17	0.0444 (16)	0.0420 (15)	0.0262 (13)	−0.0195 (13)	−0.0159 (12)	0.0057 (11)
C18	0.0384 (15)	0.0445 (15)	0.0243 (13)	−0.0179 (12)	−0.0138 (11)	0.0045 (11)
C19	0.065 (2)	0.0474 (16)	0.0289 (15)	−0.0258 (15)	−0.0159 (14)	0.0046 (12)
C20	0.082 (2)	0.0429 (17)	0.0404 (17)	−0.0256 (16)	−0.0196 (17)	0.0082 (13)
C21	0.067 (2)	0.0583 (19)	0.0350 (16)	−0.0330 (17)	−0.0186 (15)	0.0178 (14)
C22	0.0548 (19)	0.065 (2)	0.0235 (14)	−0.0287 (16)	−0.0106 (13)	0.0070 (13)
C23	0.0480 (17)	0.0463 (16)	0.0287 (14)	−0.0208 (13)	−0.0130 (13)	0.0023 (11)
C102	0.0517 (18)	0.0476 (16)	0.0296 (14)	−0.0157 (14)	−0.0125 (13)	−0.0044 (12)
O101	0.0537 (12)	0.0380 (10)	0.0212 (9)	−0.0140 (9)	−0.0151 (8)	0.0005 (7)
O171	0.0739 (14)	0.0467 (12)	0.0284 (10)	−0.0295 (10)	−0.0194 (10)	0.0076 (8)

Geometric parameters (Å, °)

S1—O2	1.425 (2)	C12—C13	1.392 (4)
S1—O1	1.4280 (19)	C12—H12	0.9300
S1—N1	1.621 (2)	C13—C14	1.386 (3)
S1—C9	1.770 (2)	C13—C15	1.462 (3)
N1—C2	1.464 (4)	C14—H14	0.9300
N1—H1	0.84 (3)	C15—C16	1.322 (4)
C2—C3	1.505 (4)	C15—H15	0.9300
C2—H2A	0.9700	C16—C17	1.471 (3)
C2—H2B	0.9700	C16—H16	0.9300
C3—C4	1.371 (4)	C17—O171	1.219 (3)
C3—C8	1.390 (4)	C17—C18	1.496 (4)
C4—C5	1.389 (5)	C18—C19	1.378 (4)
C4—H4	0.9300	C18—C23	1.388 (3)
C5—C6	1.380 (5)	C19—C20	1.384 (4)
C5—H5	0.9300	C19—H19	0.9300
C6—C7	1.369 (5)	C20—C21	1.374 (4)
C6—H6	0.9300	C20—H20	0.9300
C7—C8	1.378 (4)	C21—C22	1.364 (4)
C7—H7	0.9300	C21—H21	0.9300
C8—H8	0.9300	C22—C23	1.375 (4)
C9—C14	1.394 (3)	C22—H22	0.9300
C9—C10	1.398 (3)	C23—H23	0.9300
C10—O101	1.350 (3)	C102—O101	1.430 (3)
C10—C11	1.390 (3)	C102—H10A	0.9600
C11—C12	1.376 (4)	C102—H10B	0.9600

C11—H11	0.9300	C102—H10C	0.9600
O2—S1—O1	119.04 (12)	C11—C12—H12	118.7
O2—S1—N1	107.38 (12)	C13—C12—H12	118.7
O1—S1—N1	107.21 (12)	C14—C13—C12	117.3 (2)
O2—S1—C9	110.21 (12)	C14—C13—C15	119.6 (2)
O1—S1—C9	105.83 (11)	C12—C13—C15	123.0 (2)
N1—S1—C9	106.50 (12)	C13—C14—C9	121.4 (2)
C2—N1—S1	117.40 (18)	C13—C14—H14	119.3
C2—N1—H1	115 (2)	C9—C14—H14	119.3
S1—N1—H1	110 (2)	C16—C15—C13	126.7 (3)
N1—C2—C3	113.2 (2)	C16—C15—H15	116.7
N1—C2—H2A	108.9	C13—C15—H15	116.7
C3—C2—H2A	108.9	C15—C16—C17	121.9 (3)
N1—C2—H2B	108.9	C15—C16—H16	119.0
C3—C2—H2B	108.9	C17—C16—H16	119.0
H2A—C2—H2B	107.8	O171—C17—C16	120.9 (2)
C4—C3—C8	118.5 (3)	O171—C17—C18	120.2 (2)
C4—C3—C2	119.1 (3)	C16—C17—C18	118.9 (2)
C8—C3—C2	122.3 (3)	C19—C18—C23	118.8 (2)
C3—C4—C5	121.2 (3)	C19—C18—C17	123.1 (2)
C3—C4—H4	119.4	C23—C18—C17	118.0 (2)
C5—C4—H4	119.4	C18—C19—C20	120.4 (3)
C6—C5—C4	119.5 (3)	C18—C19—H19	119.8
C6—C5—H5	120.2	C20—C19—H19	119.8
C4—C5—H5	120.2	C21—C20—C19	120.0 (3)
C7—C6—C5	119.7 (3)	C21—C20—H20	120.0
C7—C6—H6	120.2	C19—C20—H20	120.0
C5—C6—H6	120.2	C22—C21—C20	120.1 (3)
C6—C7—C8	120.6 (3)	C22—C21—H21	119.9
C6—C7—H7	119.7	C20—C21—H21	119.9
C8—C7—H7	119.7	C21—C22—C23	120.3 (3)
C7—C8—C3	120.4 (3)	C21—C22—H22	119.9
C7—C8—H8	119.8	C23—C22—H22	119.9
C3—C8—H8	119.8	C22—C23—C18	120.4 (3)
C14—C9—C10	119.9 (2)	C22—C23—H23	119.8
C14—C9—S1	118.77 (19)	C18—C23—H23	119.8
C10—C9—S1	121.27 (18)	O101—C102—H10A	109.5
O101—C10—C11	124.1 (2)	O101—C102—H10B	109.5
O101—C10—C9	116.9 (2)	H10A—C102—H10B	109.5
C11—C10—C9	119.0 (2)	O101—C102—H10C	109.5
C12—C11—C10	119.8 (2)	H10A—C102—H10C	109.5
C12—C11—H11	120.1	H10B—C102—H10C	109.5
C10—C11—H11	120.1	C10—O101—C102	117.8 (2)
C11—C12—C13	122.5 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O171^{i}	0.84 (3)	2.23 (3)	3.018 (3)	156 (3)

Symmetry codes: (i) *x*, *y*, *z*−1.

Fig. 1

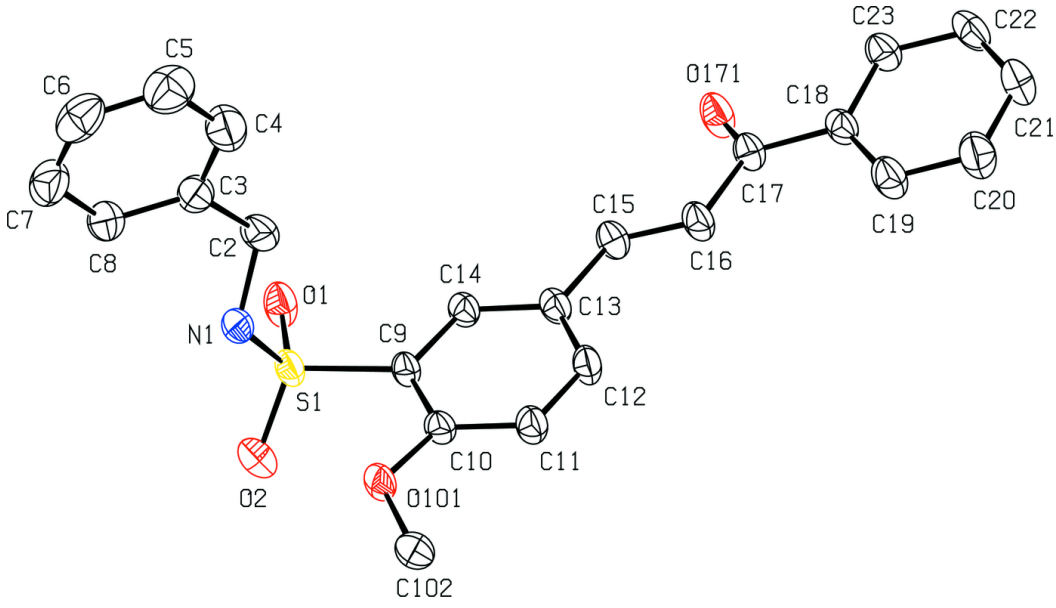

Fig. 2