

(2E)-1-(5-Bromothiophen-2-yl)-3-(2,3,4-trimethoxyphenyl)prop-2-en-1-one

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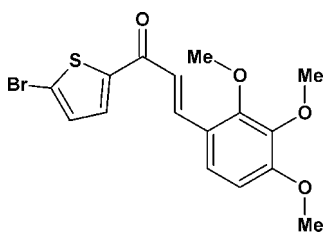
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.033; wR factor = 0.082; data-to-parameter ratio = 14.0.

In the title compound, $\text{C}_{16}\text{H}_{15}\text{BrO}_4\text{S}$, the thiophene ring is not coplanar with the benzene ring; the dihedral angle between the two planes is $11.08(12)^\circ$. The crystal structure is characterized by $\text{C}-\text{H}\cdots\text{O}$ interactions. Weak intramolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds also occur.

Related literature

For general background to chalcones, see: Chun *et al.* (2001); Horng *et al.* (2003); Lopez *et al.* (2001); Zubieta *et al.* (2001); Howard *et al.* (2004); Petrash (2004); Lu *et al.* (2010). Mei *et al.* (2003). For related structures, see: Liang *et al.* (2011); Alex *et al.* (1993); Li & Su (1993).



Experimental

Crystal data

 $\text{C}_{16}\text{H}_{15}\text{BrO}_4\text{S}$ $M_r = 383.25$ Monoclinic, $P2_1/c$ $a = 8.114(5)$ Å $b = 12.775(5)$ Å $c = 15.404(5)$ Å $\beta = 98.813(5)^\circ$ $V = 1577.9(13)$ Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 2.75$ mm⁻¹ $T = 293$ K $0.22 \times 0.15 \times 0.12$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer

Absorption correction: multi-scan (*CrysAlis PRO RED*; OxfordDiffraction, 2010)
 $T_{\min} = 0.228$, $T_{\max} = 1.000$
16471 measured reflections2784 independent reflections
2343 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.042$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.033$ $wR(F^2) = 0.082$ $S = 1.06$

2784 reflections

199 parameters

H-atom parameters constrained

 $\Delta\rho_{\max} = 0.33$ e Å⁻³ $\Delta\rho_{\min} = -0.59$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C8}-\text{H8B}\cdots\text{O5}$	0.96	2.23	2.861 (4)	122
$\text{C9}-\text{H9B}\cdots\text{O4}$	0.96	2.38	2.985 (4)	120
$\text{C21}-\text{H21}\cdots\text{O6}^i$	0.93	2.41	3.322 (4)	165

Symmetry code: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$.

Data collection: *CrysAlis PRO CCD* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO CCD*; data reduction: *CrysAlis PRO RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2039).

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supplementary materials

Acta Cryst. (2012). E68, o61 [doi:10.1107/S1600536811052202]

(2E)-1-(5-Bromothiophen-2-yl)-3-(2,3,4-trimethoxyphenyl)prop-2-en-1-one

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Comment

Chalcones are alpha, beta unsaturated ketones, widely distributed in nature and are extensively studied for their biological activity (Chun *et al.*, 2001; Horng *et al.*, 2003; Lopez *et al.*, 2001; Mei *et al.*, 2003). Chalcones readily crystallize because of their intermolecular hydrogen bonding (Liang *et al.*, 2011; Alex *et al.*, 1993; Li *et al.*, 1993). The same property has been shown to be responsible for its biological activity (Zubieta *et al.*, 2001). However, halogen containing chalcones are of special interest in drug design process because of the raising importance of hydrogen bond contribution in target recognition process (Howard *et al.*, 2004; Petrash, 2004; Lu *et al.*, 2010). Crystal structure conformation of small molecule has always been the choice for binding energy calculations in docking studies. In this paper we report the crystal structure of (2E)-1-(5-bromothiophen-2-yl)-3-(2,3,4-trimethoxyphenyl)prop-2-en-1-one which is a part of insilico lead identification studies.

The asymmetric unit of (2E)-1-(5-bromothiophen-2-yl)-3-(2,3,4-trimethoxyphenyl)prop-2-en-1-one, C₁₆H₁₅BrO₄S, contains just one molecule (Fig. 1). The five-membered thiophene ring (S2\C19...C22) is not coplanar with the phenyl ring (C10\C11...C15) system; the dihedral angle between the two planes is 11.08 (12)°. The crystal structure displays intermolecular C21—H21...O6 and weak intramolecular C8—H8B...O5 and C9—H9B...O4 hydrogen bonds (Table 1). The packing of molecules in the crystal structure is depicted in Fig. 2.

Experimental

A mixture of 2-acetyl-5-BromoThiophene (0.01 mole) and 2,3,4-trimethoxybenzaldehyde (0.01 mole) were stirred in ethanol (30 ml) and then an aqueous solution of potassium hydroxide (40%, 15 ml) was added to it. The mixture was kept overnight at room temperature and then it was poured into crushed ice and acidified with dilute hydrochloric acid. The precipitated chalcone was filtered and crystallized from ethanol.

Refinement

All H atoms were positioned at calculated positions C—H = 0.93 Å for aromatic H and C—H = 0.96 Å for methyl H and refined using a riding model with $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic and $U_{iso}(H) = 1.2U_{eq}(C)$ for methyl H.

Figures

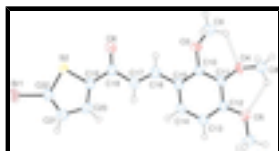


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. The H atoms are shown as spheres of arbitrary radii. The dashed line indicates the intramolecular hydrogen bond.

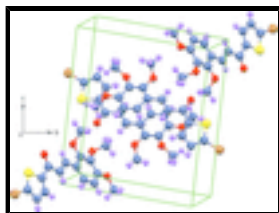


Fig. 2. Packing of the molecules.

(2E)-1-(5-Bromothiophen-2-yl)-3-(2,3,4-trimethoxyphenyl)prop-2-en-1-one

Crystal data

$C_{16}H_{15}BrO_4S$

$M_r = 383.25$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 8.114$ (5) Å

$b = 12.775$ (5) Å

$c = 15.404$ (5) Å

$\beta = 98.813$ (5)°

$V = 1577.9$ (13) Å³

$Z = 4$

$F(000) = 776$

$D_x = 1.613$ Mg m⁻³

Melting point: 400 K

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2784 reflections

$\theta = 2.5$ – 25.0°

$\mu = 2.75$ mm⁻¹

$T = 293$ K

Prism, colourless

$0.22 \times 0.15 \times 0.12$ mm

Data collection

Oxford Diffraction Xcalibur
diffractometer

Radiation source: fine-focus sealed tube
graphite

Detector resolution: 16.0839 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(*CrysAlis PRO RED*; Oxford Diffraction, 2010)

$T_{\min} = 0.228$, $T_{\max} = 1.000$

16471 measured reflections

2784 independent reflections

2343 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.042$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.5^\circ$

$h = -9 \rightarrow 9$

$k = -15 \rightarrow 15$

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.033$

$wR(F^2) = 0.082$

$S = 1.06$

2784 reflections

199 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0349P)^2 + 0.9331P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.007$

$\Delta\rho_{\max} = 0.33$ e Å⁻³

0 restraints

$$\Delta\rho_{\min} = -0.59 \text{ e } \text{\AA}^{-3}$$

Special details

Experimental. *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.33.55 (release 05-01-2010 CrysAlis171. NET) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	−0.24507 (4)	0.00703 (2)	0.22076 (2)	0.05109 (14)
S2	−0.11145 (9)	0.10763 (6)	0.06120 (5)	0.03737 (19)
O3	0.3504 (3)	0.47747 (15)	−0.20529 (13)	0.0450 (5)
O4	0.5493 (2)	0.65241 (14)	−0.19864 (12)	0.0378 (5)
O5	0.5662 (2)	0.78703 (15)	−0.06147 (13)	0.0429 (5)
O6	0.0059 (3)	0.22557 (18)	−0.08036 (14)	0.0561 (6)
C7	0.5915 (4)	0.8532 (3)	0.0134 (2)	0.0527 (8)
H7A	0.6611	0.9111	0.0026	0.079*
H7B	0.6446	0.8143	0.0633	0.079*
H7C	0.4859	0.8790	0.0250	0.079*
C8	0.5199 (4)	0.7480 (2)	−0.2465 (2)	0.0566 (9)
H8A	0.5915	0.7515	−0.2906	0.085*
H8B	0.5428	0.8062	−0.2070	0.085*
H8C	0.4056	0.7507	−0.2742	0.085*
C9	0.2743 (4)	0.5175 (3)	−0.2882 (2)	0.0592 (10)
H9A	0.2735	0.4642	−0.3322	0.089*
H9B	0.3363	0.5769	−0.3036	0.089*
H9C	0.1619	0.5383	−0.2847	0.089*
C10	0.3613 (3)	0.5446 (2)	−0.13548 (17)	0.0301 (6)
C11	0.4561 (3)	0.6350 (2)	−0.13228 (17)	0.0294 (6)
C12	0.4695 (3)	0.6998 (2)	−0.05918 (17)	0.0305 (6)
C13	0.3899 (3)	0.6724 (2)	0.01106 (17)	0.0351 (6)
H13	0.3962	0.7162	0.0597	0.042*
C14	0.3017 (3)	0.5805 (2)	0.00854 (18)	0.0340 (6)
H14	0.2531	0.5616	0.0571	0.041*
C15	0.2827 (3)	0.5150 (2)	−0.06390 (18)	0.0305 (6)
C16	0.1893 (3)	0.4176 (2)	−0.06729 (19)	0.0358 (6)
H16	0.1706	0.3834	−0.1212	0.043*
C17	0.1279 (3)	0.3722 (2)	−0.00165 (19)	0.0387 (7)

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H17	0.1416	0.4057	0.0526	0.046*
C18	0.0399 (3)	0.2720 (2)	−0.01058 (19)	0.0368 (7)
C19	−0.0079 (3)	0.2265 (2)	0.06962 (18)	0.0331 (6)
C20	0.0083 (3)	0.2636 (2)	0.15283 (19)	0.0401 (7)
H20	0.0614	0.3264	0.1700	0.048*
C21	−0.0624 (4)	0.1988 (2)	0.21091 (19)	0.0419 (7)
H21	−0.0613	0.2134	0.2702	0.050*
C22	−0.1317 (3)	0.1132 (2)	0.16997 (18)	0.0363 (7)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0619 (2)	0.0412 (2)	0.0540 (2)	−0.00626 (15)	0.02110 (16)	0.01379 (15)
S2	0.0458 (4)	0.0314 (4)	0.0354 (4)	−0.0079 (3)	0.0077 (3)	0.0008 (3)
O3	0.0683 (14)	0.0315 (11)	0.0382 (12)	−0.0042 (10)	0.0176 (10)	−0.0070 (9)
O4	0.0486 (11)	0.0292 (11)	0.0407 (11)	−0.0010 (9)	0.0227 (9)	0.0033 (9)
O5	0.0549 (12)	0.0330 (12)	0.0421 (12)	−0.0122 (9)	0.0114 (9)	−0.0037 (9)
O6	0.0809 (16)	0.0551 (15)	0.0335 (12)	−0.0242 (12)	0.0124 (11)	0.0002 (11)
C7	0.059 (2)	0.0403 (19)	0.060 (2)	−0.0117 (16)	0.0121 (16)	−0.0162 (16)
C8	0.087 (3)	0.043 (2)	0.0442 (19)	−0.0002 (18)	0.0262 (18)	0.0127 (16)
C9	0.065 (2)	0.065 (2)	0.044 (2)	−0.0103 (18)	0.0000 (17)	−0.0121 (17)
C10	0.0364 (14)	0.0231 (14)	0.0320 (15)	0.0040 (11)	0.0093 (11)	0.0001 (11)
C11	0.0346 (14)	0.0260 (14)	0.0292 (14)	0.0040 (11)	0.0103 (11)	0.0053 (11)
C12	0.0336 (14)	0.0247 (14)	0.0333 (15)	0.0009 (11)	0.0058 (11)	0.0031 (12)
C13	0.0430 (16)	0.0350 (16)	0.0272 (14)	0.0009 (13)	0.0056 (12)	−0.0046 (12)
C14	0.0360 (15)	0.0367 (16)	0.0310 (15)	0.0009 (12)	0.0109 (11)	0.0057 (12)
C15	0.0296 (14)	0.0287 (15)	0.0340 (15)	0.0026 (11)	0.0073 (11)	0.0053 (12)
C16	0.0370 (15)	0.0327 (16)	0.0377 (16)	−0.0007 (12)	0.0061 (12)	0.0048 (13)
C17	0.0424 (16)	0.0383 (17)	0.0364 (16)	−0.0056 (13)	0.0093 (13)	0.0036 (13)
C18	0.0367 (15)	0.0373 (17)	0.0369 (17)	−0.0042 (12)	0.0070 (12)	0.0062 (13)
C19	0.0331 (14)	0.0303 (15)	0.0355 (16)	−0.0037 (11)	0.0036 (11)	0.0041 (12)
C20	0.0444 (16)	0.0334 (16)	0.0419 (18)	−0.0105 (13)	0.0043 (13)	−0.0023 (13)
C21	0.0514 (18)	0.0434 (18)	0.0319 (16)	−0.0024 (14)	0.0094 (13)	0.0016 (14)
C22	0.0383 (15)	0.0337 (16)	0.0386 (16)	0.0015 (12)	0.0113 (12)	0.0071 (13)

Geometric parameters (\AA , $^\circ$)

Br1—C22	1.876 (3)	C10—C11	1.384 (4)
S2—C22	1.710 (3)	C10—C15	1.407 (4)
S2—C19	1.730 (3)	C11—C12	1.388 (4)
O3—C10	1.368 (3)	C12—C13	1.387 (4)
O3—C9	1.426 (4)	C13—C14	1.372 (4)
O4—C11	1.379 (3)	C13—H13	0.9300
O4—C8	1.428 (3)	C14—C15	1.384 (4)
O5—C12	1.366 (3)	C14—H14	0.9300
O5—C7	1.419 (3)	C15—C16	1.454 (4)
O6—C18	1.222 (3)	C16—C17	1.327 (4)
C7—H7A	0.9600	C16—H16	0.9300
C7—H7B	0.9600	C17—C18	1.462 (4)

C7—H7C	0.9600	C17—H17	0.9300
C8—H8A	0.9600	C18—C19	1.470 (4)
C8—H8B	0.9600	C19—C20	1.354 (4)
C8—H8C	0.9600	C20—C21	1.404 (4)
C9—H9A	0.9600	C20—H20	0.9300
C9—H9B	0.9600	C21—C22	1.342 (4)
C9—H9C	0.9600	C21—H21	0.9300
C22—S2—C19	90.49 (13)	C14—C13—C12	119.8 (3)
C10—O3—C9	116.5 (2)	C14—C13—H13	120.1
C11—O4—C8	117.0 (2)	C12—C13—H13	120.1
C12—O5—C7	118.5 (2)	C13—C14—C15	122.2 (2)
O5—C7—H7A	109.5	C13—C14—H14	118.9
O5—C7—H7B	109.5	C15—C14—H14	118.9
H7A—C7—H7B	109.5	C14—C15—C10	117.5 (2)
O5—C7—H7C	109.5	C14—C15—C16	122.6 (2)
H7A—C7—H7C	109.5	C10—C15—C16	119.9 (2)
H7B—C7—H7C	109.5	C17—C16—C15	126.9 (3)
O4—C8—H8A	109.5	C17—C16—H16	116.5
O4—C8—H8B	109.5	C15—C16—H16	116.5
H8A—C8—H8B	109.5	C16—C17—C18	123.1 (3)
O4—C8—H8C	109.5	C16—C17—H17	118.5
H8A—C8—H8C	109.5	C18—C17—H17	118.5
H8B—C8—H8C	109.5	O6—C18—C17	123.3 (3)
O3—C9—H9A	109.5	O6—C18—C19	119.6 (3)
O3—C9—H9B	109.5	C17—C18—C19	117.1 (3)
H9A—C9—H9B	109.5	C20—C19—C18	131.0 (3)
O3—C9—H9C	109.5	C20—C19—S2	110.7 (2)
H9A—C9—H9C	109.5	C18—C19—S2	118.2 (2)
H9B—C9—H9C	109.5	C19—C20—C21	114.0 (3)
O3—C10—C11	121.3 (2)	C19—C20—H20	123.0
O3—C10—C15	117.7 (2)	C21—C20—H20	123.0
C11—C10—C15	120.8 (2)	C22—C21—C20	111.3 (3)
O4—C11—C10	118.2 (2)	C22—C21—H21	124.3
O4—C11—C12	121.4 (2)	C20—C21—H21	124.3
C10—C11—C12	120.0 (2)	C21—C22—S2	113.4 (2)
O5—C12—C13	124.3 (2)	C21—C22—Br1	126.2 (2)
O5—C12—C11	116.1 (2)	S2—C22—Br1	120.36 (16)
C13—C12—C11	119.6 (2)		
C9—O3—C10—C11	−63.9 (3)	O3—C10—C15—C16	−2.1 (4)
C9—O3—C10—C15	120.7 (3)	C11—C10—C15—C16	−177.5 (2)
C8—O4—C11—C10	123.4 (3)	C14—C15—C16—C17	−8.3 (4)
C8—O4—C11—C12	−63.4 (3)	C10—C15—C16—C17	170.2 (3)
O3—C10—C11—O4	−4.4 (4)	C15—C16—C17—C18	−178.0 (3)
C15—C10—C11—O4	170.9 (2)	C16—C17—C18—O6	−5.1 (5)
O3—C10—C11—C12	−177.7 (2)	C16—C17—C18—C19	174.6 (3)
C15—C10—C11—C12	−2.5 (4)	O6—C18—C19—C20	−176.7 (3)
C7—O5—C12—C13	1.7 (4)	C17—C18—C19—C20	3.6 (4)
C7—O5—C12—C11	−176.7 (2)	O6—C18—C19—S2	−0.1 (4)

supplementary materials

O4—C11—C12—O5	6.6 (4)	C17—C18—C19—S2	−179.73 (19)
C10—C11—C12—O5	179.7 (2)	C22—S2—C19—C20	0.8 (2)
O4—C11—C12—C13	−172.0 (2)	C22—S2—C19—C18	−176.6 (2)
C10—C11—C12—C13	1.2 (4)	C18—C19—C20—C21	176.4 (3)
O5—C12—C13—C14	−177.0 (2)	S2—C19—C20—C21	−0.5 (3)
C11—C12—C13—C14	1.4 (4)	C19—C20—C21—C22	−0.2 (4)
C12—C13—C14—C15	−2.8 (4)	C20—C21—C22—S2	0.8 (3)
C13—C14—C15—C10	1.5 (4)	C20—C21—C22—Br1	−178.3 (2)
C13—C14—C15—C16	−179.9 (2)	C19—S2—C22—C21	−0.9 (2)
O3—C10—C15—C14	176.5 (2)	C19—S2—C22—Br1	178.24 (17)
C11—C10—C15—C14	1.1 (4)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8—H8B \cdots O5	0.96	2.23	2.861 (4)	122.
C9—H9B \cdots O4	0.96	2.38	2.985 (4)	120.
C21—H21 \cdots O6 ⁱ	0.93	2.41	3.322 (4)	165.

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

Fig. 1

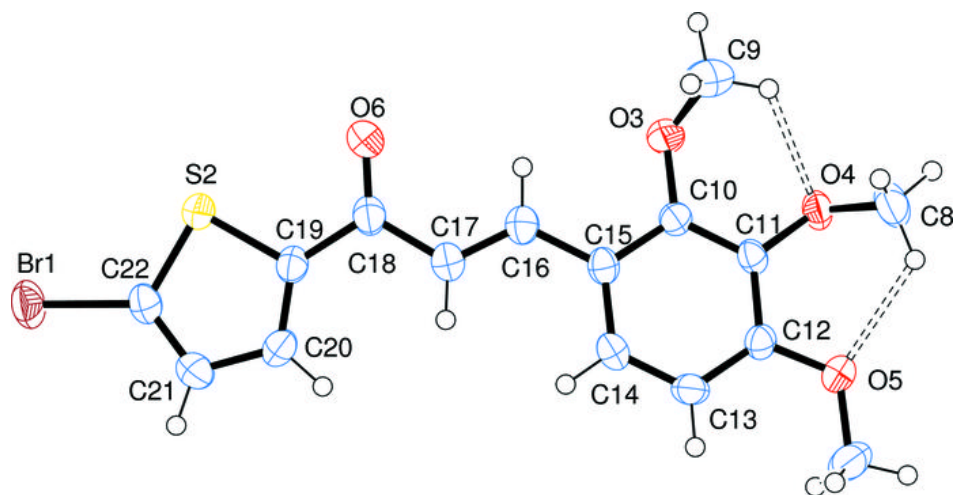


Fig. 2

