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6-(2,6-Dichlorobenzyl)-5-ethyl-2-(4-methoxybenzylsulfanyl)pyrimidin-4(3*H*)-one

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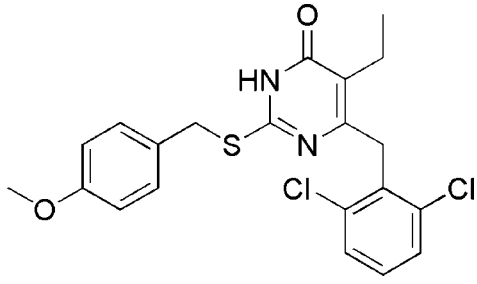
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.069; wR factor = 0.222; data-to-parameter ratio = 18.3.

The title compound, $C_{21}H_{20}Cl_2N_2O_2S$, was synthesized as a potential reverse transcriptase (RT) inhibitor of the human immunodeficiency virus type 1 (HIV-1). Structural analysis confirms that the compound is present in the 3*H*-tautomeric form. A centrosymmetric dimer is formed in the crystal structure through pairs of N—H···O hydrogen bonds. The structure also displays C—H···Cl and C—H···O interactions.

Related literature

For the crystal structure of a related pyrimidin-4(3*H*)-one, see: Ji *et al.* (2006).



Experimental

Crystal data

$C_{21}H_{20}Cl_2N_2O_2S$
M_r = 435.35
Monoclinic, $P2_1/c$
a = 10.037 (3) Å
b = 17.264 (5) Å
c = 13.006 (4) Å
β = 105.901 (5)°
V = 2167.4 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.42 mm^{-1}
T = 293 (2) K
0.20 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.922, T_{max} = 0.940
10682 measured reflections
4733 independent reflections
2050 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.222
S = 0.87
4733 reflections
259 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15*B*···Cl1	0.97	2.56	3.043 (4)	111
C7—H7···O1^{i}	0.93	2.49	3.389 (5)	162
N1—H1···O2^{ii}	0.858 (10)	1.921 (11)	2.777 (4)	175 (3)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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, 2000); 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: RZ2158).

References

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Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

  doi:10.1107/S1600536807034976

supplementary materials

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6-(2,6-Dichlorobenzyl)-5-ethyl-2-(4-methoxybenzylsulfanyl)pyrimidin-4(3*H*)-one

Y.-P. Wang, F.-E. Chen and M.-Q. Chen

Comment

As part of an ongoing research work aimed at developing potent HIV-1 inhibitors, we have recently focused our attention on the structural modifications of dihydroalkoxybenzyloxopyrimidines (DABOs), one of the most interesting and representative classes of non-nucleoside reverse transcriptase inhibitors (NNRTIs). We have synthesized a series of 2-arylalkylsulfur-substituted DABOs analogues, including the title compound, (I), as potential HIV-1 inhibitors. According to the possible delocalization of the C═N double bond in the pyrimidine ring, compound (I) could theoretically exist in three different tautomeric forms: the 1*H*-, the 3*H*-, and the aromatic form (Fig. 1). While NMR spectroscopy strongly indicated that the title compound adopted the 3*H*-tautomeric form, confirmations was sought using X-ray crystallography.

In the structure of (I), the carbonyl C—O bond length is 1.245 (4) Å, which is not significantly different from the value of 1.242 (3) Å found in 2-(cyclopentylsulfanyl)-6-(1-naphthoyl)-pyrimidin-4(3*H*)-one (Ji *et al.*, 2006). Meanwhile, the lengths of C9—N1 and C9—N2 bonds are 1.344 (4) Å and 1.299 (4) Å, respectively. These values confirm that the title compound adopts the 3*H*-tautomeric form in the solid state (Fig. 2).

In the crystal structure, centrosymmetric dimers are formed by pairs of N1—H1···O2^{ii} hydrogen bonds [symmetry code: (ii) −*x*, −*y* + 2, −*z*]. These dimers are further linked by weak C—H···O interactions (Table 1, Fig. 3).

Experimental

To a stirred solution of 6-(2,6-dichlorobenzyl)-5-ethyl-2,3-dihydro-2-thioxopyrimidin-4(1*H*)-one (1 g, 3.17 mmol) in anhydrous DMF (18 ml) was added K_2CO_3 (0.53 g, 3.84 mmol) under a nitrogen atmosphere. The mixture was stirred at 298 K for 20 min, then 1-(bromomethyl)-4-methoxybenzene (0.60 g, 3.83 mmol) was added, and the reaction mixture was stirred at 298 K for 28 h. The reaction mixture was poured into cold H_2O (100 ml), the resulting precipitate was collected by filtration, washed with water and recrystallized from butan-2-one (yield: 46%; m.p. 504.2–504.5 K). Single cystals of the title compound suitable for X-ray diffraction were grown by slow evaporation of a DMF solution. The product was characterized by IR, MS, ^{1}H NMR and ^{13}C NMR.

Refinement

The H atom bound to N1 was located in a difference Fourier map and refined with a distance restraint of 0.86 (1) Å. All other H atoms were placed in geometrically idealized position and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å, and with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for other H atoms. Methyl groups were allowed to rotate freely about the C—C bond.

Figures

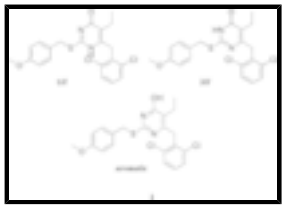


Fig. 1. Possible tautomeric forms of the title compound.

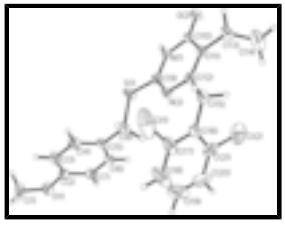


Fig. 2. The molecular structure of the title compound showing 30% probability of displacement ellipsoids and the atom-numbering scheme.

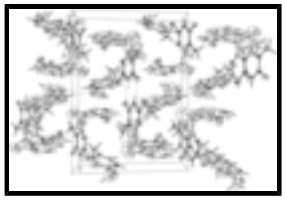


Fig. 3. Packing diagram of the title compound viewed along the *a* axis. Thermal ellipsoids are drawn at the 30% probability level. Intermolecular N—H···O hydrogen bonds are shown as dashed lines.

6-(2,6-Dichlorobenzyl)-5-ethyl-2-(4-methoxybenzylsulfanyl)pyrimidin-4(3*H*)-one

Crystal data

$C_{21}H_{20}Cl_2N_2O_2S$	F_{000} = 904
M_r = 435.35	D_x = 1.334 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 946 reflections
a = 10.037 (3) Å	θ = 2.4–19.2º
b = 17.264 (5) Å	μ = 0.42 mm^{-1}
c = 13.006 (4) Å	T = 293 (2) K
β = 105.901 (5)º	Block, colourless
V = 2167.4 (12) Å^3	0.20 × 0.20 × 0.15 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	4733 independent reflections
Radiation source: fine-focus sealed tube	2050 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.050
T = 293(2) K	θ_{max} = 27.2º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −12→12

T_{min} = 0.922, T_{max} = 0.940	k = −21→21
10682 measured reflections	l = −14→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.069	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.222	$w = 1/[\sigma^2(F_o^2) + (0.1246P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.87	$(\Delta/\sigma)_{max} < 0.001$
4733 reflections	$\Delta\rho_{max}$ = 0.79 e Å^{-3}
259 parameters	$\Delta\rho_{min}$ = −0.36 e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
Cl1	0.4124 (2)	0.63842 (15)	−0.0284 (2)	0.2158 (13)
Cl2	0.1444 (2)	0.68614 (13)	0.26805 (15)	0.1606 (8)
N1	0.1198 (3)	0.92035 (15)	0.0294 (2)	0.0535 (7)
N2	0.2527 (3)	0.80811 (15)	0.0714 (2)	0.0565 (7)
O1	1.0343 (3)	1.00550 (19)	0.3657 (2)	0.0954 (10)
O2	−0.1101 (2)	0.92001 (13)	−0.05248 (19)	0.0621 (7)
S1	0.38515 (10)	0.94244 (5)	0.11803 (10)	0.0775 (4)
C1	1.1372 (5)	1.0113 (4)	0.3105 (4)	0.145 (3)
H1A	1.1553	0.9609	0.2861	0.217*
H1B	1.2207	1.0318	0.3576	0.217*
H1C	1.1055	1.0452	0.2502	0.217*
C2	0.9086 (4)	0.9743 (2)	0.3126 (3)	0.0639 (10)
C3	0.8719 (4)	0.9551 (3)	0.2074 (3)	0.0863 (13)
H3	0.9330	0.9639	0.1662	0.104*

C4	0.7439 (4)	0.9227 (3)	0.1616 (3)	0.0837 (13)
H4	0.7197	0.9098	0.0894	0.100*
C5	0.6523 (4)	0.9091 (2)	0.2194 (3)	0.0645 (10)
C6	0.6893 (4)	0.9330 (2)	0.3243 (3)	0.0652 (10)
H6	0.6264	0.9274	0.3646	0.078*
C7	0.8158 (4)	0.9646 (2)	0.3704 (3)	0.0649 (10)
H7	0.8387	0.9796	0.4418	0.078*
C8	0.5162 (4)	0.8701 (2)	0.1694 (4)	0.0775 (12)
H8A	0.4898	0.8385	0.2222	0.093*
H8B	0.5250	0.8366	0.1117	0.093*
C9	0.2405 (3)	0.88306 (18)	0.0689 (3)	0.0545 (9)
C10	−0.0018 (3)	0.88240 (18)	−0.0153 (3)	0.0519 (8)
C11	0.0061 (3)	0.79882 (18)	−0.0140 (3)	0.0529 (8)
C12	0.1330 (4)	0.76667 (18)	0.0313 (3)	0.0523 (8)
C13	−0.1228 (4)	0.7540 (2)	−0.0637 (4)	0.0788 (12)
H13A	−0.1796	0.7836	−0.1230	0.095*
H13B	−0.0974	0.7061	−0.0925	0.095*
C14	−0.2057 (6)	0.7353 (4)	0.0102 (6)	0.149 (3)
H14A	−0.1524	0.7031	0.0669	0.223*
H14B	−0.2881	0.7082	−0.0277	0.223*
H14C	−0.2307	0.7823	0.0397	0.223*
C15	0.1547 (4)	0.67980 (19)	0.0402 (3)	0.0621 (10)
H15A	0.0758	0.6558	0.0569	0.074*
H15B	0.1605	0.6595	−0.0280	0.074*
C16	0.2846 (4)	0.65926 (18)	0.1253 (4)	0.0668 (11)
C17	0.4062 (5)	0.6412 (3)	0.1025 (6)	0.111 (2)
C18	0.5284 (9)	0.6259 (5)	0.1810 (11)	0.179 (5)
H18	0.6096	0.6135	0.1633	0.215*
C19	0.5249 (13)	0.6295 (5)	0.2816 (12)	0.202 (7)
H19	0.6067	0.6211	0.3350	0.242*
C20	0.4118 (10)	0.6443 (4)	0.3100 (7)	0.168 (4)
H20	0.4137	0.6429	0.3818	0.202*
C21	0.2899 (6)	0.6619 (3)	0.2338 (5)	0.1020 (16)
H1	0.112 (3)	0.9696 (6)	0.034 (2)	0.052 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.178 (2)	0.227 (2)	0.307 (3)	−0.0219 (17)	0.177 (2)	−0.089 (2)
Cl2	0.1943 (19)	0.1909 (17)	0.1253 (14)	−0.0393 (15)	0.0923 (13)	−0.0251 (12)
N1	0.0436 (17)	0.0386 (15)	0.072 (2)	−0.0006 (12)	0.0052 (14)	−0.0033 (14)
N2	0.0438 (16)	0.0430 (15)	0.076 (2)	−0.0018 (12)	0.0059 (14)	0.0002 (14)
O1	0.0632 (18)	0.143 (3)	0.0700 (18)	−0.0409 (18)	0.0010 (14)	0.0038 (18)
O2	0.0438 (14)	0.0544 (14)	0.0789 (17)	0.0035 (11)	0.0011 (12)	−0.0029 (12)
S1	0.0474 (6)	0.0494 (5)	0.1179 (9)	−0.0064 (4)	−0.0075 (5)	−0.0015 (5)
C1	0.068 (3)	0.265 (8)	0.099 (4)	−0.071 (4)	0.019 (3)	0.014 (5)
C2	0.050 (2)	0.080 (2)	0.054 (2)	−0.0116 (19)	0.0014 (17)	0.0017 (19)
C3	0.063 (3)	0.133 (4)	0.063 (3)	−0.020 (3)	0.019 (2)	−0.011 (3)

C4	0.063 (3)	0.124 (4)	0.057 (2)	−0.011 (3)	0.003 (2)	−0.022 (2)
C5	0.043 (2)	0.061 (2)	0.081 (3)	−0.0001 (16)	0.0021 (19)	−0.002 (2)
C6	0.050 (2)	0.072 (2)	0.072 (3)	0.0005 (18)	0.0140 (19)	0.009 (2)
C7	0.063 (2)	0.074 (2)	0.053 (2)	−0.0082 (19)	0.0096 (19)	−0.0013 (19)
C8	0.046 (2)	0.060 (2)	0.109 (3)	0.0023 (18)	−0.008 (2)	0.000 (2)
C9	0.045 (2)	0.0464 (19)	0.067 (2)	−0.0030 (15)	0.0074 (16)	−0.0016 (16)
C10	0.043 (2)	0.0508 (19)	0.059 (2)	−0.0008 (16)	0.0085 (16)	−0.0040 (16)
C11	0.0436 (19)	0.0478 (18)	0.064 (2)	−0.0055 (15)	0.0087 (16)	−0.0037 (16)
C12	0.052 (2)	0.0465 (17)	0.059 (2)	−0.0032 (15)	0.0162 (17)	−0.0041 (16)
C13	0.046 (2)	0.057 (2)	0.126 (4)	−0.0074 (18)	0.010 (2)	−0.005 (2)
C14	0.100 (5)	0.131 (5)	0.224 (8)	−0.029 (4)	0.060 (5)	−0.040 (5)
C15	0.061 (2)	0.0440 (18)	0.080 (3)	−0.0027 (16)	0.019 (2)	−0.0100 (18)
C16	0.054 (2)	0.0361 (17)	0.106 (3)	0.0002 (16)	0.014 (2)	0.003 (2)
C17	0.061 (3)	0.065 (3)	0.212 (7)	0.006 (2)	0.045 (4)	−0.005 (3)
C18	0.072 (5)	0.086 (4)	0.365 (16)	0.023 (3)	0.038 (9)	0.009 (8)
C19	0.123 (8)	0.083 (5)	0.333 (17)	−0.010 (5)	−0.050 (12)	0.077 (9)
C20	0.168 (7)	0.129 (6)	0.151 (6)	−0.046 (6)	−0.050 (7)	0.068 (5)
C21	0.117 (4)	0.079 (3)	0.094 (4)	−0.025 (3)	0.000 (3)	0.022 (3)

Geometric parameters (Å, °)

Cl1—C17	1.720 (7)	C7—H7	0.9300
Cl2—C21	1.692 (6)	C8—H8A	0.9700
N1—C9	1.344 (4)	C8—H8B	0.9700
N1—C10	1.366 (4)	C10—C11	1.445 (4)
N1—H1	0.858 (10)	C11—C12	1.367 (5)
N2—C9	1.299 (4)	C11—C13	1.494 (5)
N2—C12	1.372 (4)	C12—C15	1.515 (5)
O1—C2	1.372 (4)	C13—C14	1.470 (7)
O1—C1	1.414 (5)	C13—H13A	0.9700
O2—C10	1.245 (4)	C13—H13B	0.9700
S1—C9	1.749 (3)	C14—H14A	0.9600
S1—C8	1.804 (4)	C14—H14B	0.9600
C1—H1A	0.9600	C14—H14C	0.9600
C1—H1B	0.9600	C15—C16	1.504 (5)
C1—H1C	0.9600	C15—H15A	0.9700
C2—C3	1.357 (5)	C15—H15B	0.9700
C2—C7	1.358 (5)	C16—C17	1.369 (6)
C3—C4	1.378 (5)	C16—C21	1.398 (6)
C3—H3	0.9300	C17—C18	1.390 (11)
C4—C5	1.358 (5)	C18—C19	1.320 (15)
C4—H4	0.9300	C18—H18	0.9300
C5—C6	1.375 (5)	C19—C20	1.311 (13)
C5—C8	1.501 (5)	C19—H19	0.9300
C6—C7	1.361 (5)	C20—C21	1.381 (9)
C6—H6	0.9300	C20—H20	0.9300
C9—N1—C10	122.6 (3)	C12—C11—C10	116.9 (3)
C9—N1—H1	123 (2)	C12—C11—C13	124.8 (3)
C10—N1—H1	115 (2)	C10—C11—C13	118.3 (3)

C9—N2—C12	116.3 (3)	C11—C12—N2	124.6 (3)
C2—O1—C1	118.1 (3)	C11—C12—C15	122.1 (3)
C9—S1—C8	100.25 (17)	N2—C12—C15	113.3 (3)
O1—C1—H1A	109.5	C14—C13—C11	114.1 (4)
O1—C1—H1B	109.5	C14—C13—H13A	108.7
H1A—C1—H1B	109.5	C11—C13—H13A	108.7
O1—C1—H1C	109.5	C14—C13—H13B	108.7
H1A—C1—H1C	109.5	C11—C13—H13B	108.7
H1B—C1—H1C	109.5	H13A—C13—H13B	107.6
C3—C2—C7	119.4 (4)	C13—C14—H14A	109.5
C3—C2—O1	124.1 (3)	C13—C14—H14B	109.5
C7—C2—O1	116.5 (3)	H14A—C14—H14B	109.5
C2—C3—C4	119.8 (4)	C13—C14—H14C	109.5
C2—C3—H3	120.1	H14A—C14—H14C	109.5
C4—C3—H3	120.1	H14B—C14—H14C	109.5
C5—C4—C3	121.6 (4)	C16—C15—C12	111.5 (3)
C5—C4—H4	119.2	C16—C15—H15A	109.3
C3—C4—H4	119.2	C12—C15—H15A	109.3
C4—C5—C6	117.2 (3)	C16—C15—H15B	109.3
C4—C5—C8	120.7 (4)	C12—C15—H15B	109.3
C6—C5—C8	122.1 (4)	H15A—C15—H15B	108.0
C7—C6—C5	121.6 (3)	C17—C16—C21	115.9 (5)
C7—C6—H6	119.2	C17—C16—C15	122.6 (5)
C5—C6—H6	119.2	C21—C16—C15	121.4 (4)
C2—C7—C6	120.3 (4)	C16—C17—C18	122.9 (7)
C2—C7—H7	119.9	C16—C17—Cl1	119.8 (5)
C6—C7—H7	119.9	C18—C17—Cl1	117.2 (6)
C5—C8—S1	109.6 (3)	C19—C18—C17	117.5 (11)
C5—C8—H8A	109.8	C19—C18—H18	121.3
S1—C8—H8A	109.8	C17—C18—H18	121.3
C5—C8—H8B	109.8	C20—C19—C18	123.2 (13)
S1—C8—H8B	109.8	C20—C19—H19	118.4
H8A—C8—H8B	108.2	C18—C19—H19	118.4
N2—C9—N1	123.8 (3)	C19—C20—C21	120.5 (11)
N2—C9—S1	120.7 (3)	C19—C20—H20	119.8
N1—C9—S1	115.5 (2)	C21—C20—H20	119.8
O2—C10—N1	119.9 (3)	C20—C21—C16	119.8 (7)
O2—C10—C11	124.4 (3)	C20—C21—Cl2	121.7 (6)
N1—C10—C11	115.7 (3)	C16—C21—Cl2	118.5 (4)
C1—O1—C2—C3	−6.3 (7)	C10—C11—C12—N2	−2.6 (5)
C1—O1—C2—C7	175.5 (5)	C13—C11—C12—N2	176.1 (3)
C7—C2—C3—C4	−3.1 (7)	C10—C11—C12—C15	178.5 (3)
O1—C2—C3—C4	178.7 (4)	C13—C11—C12—C15	−2.9 (5)
C2—C3—C4—C5	−0.1 (7)	C9—N2—C12—C11	2.8 (5)
C3—C4—C5—C6	3.6 (7)	C9—N2—C12—C15	−178.1 (3)
C3—C4—C5—C8	−177.0 (4)	C12—C11—C13—C14	91.8 (5)
C4—C5—C6—C7	−4.0 (6)	C10—C11—C13—C14	−89.6 (5)
C8—C5—C6—C7	176.6 (3)	C11—C12—C15—C16	−159.2 (3)
C3—C2—C7—C6	2.7 (6)	N2—C12—C15—C16	21.7 (4)

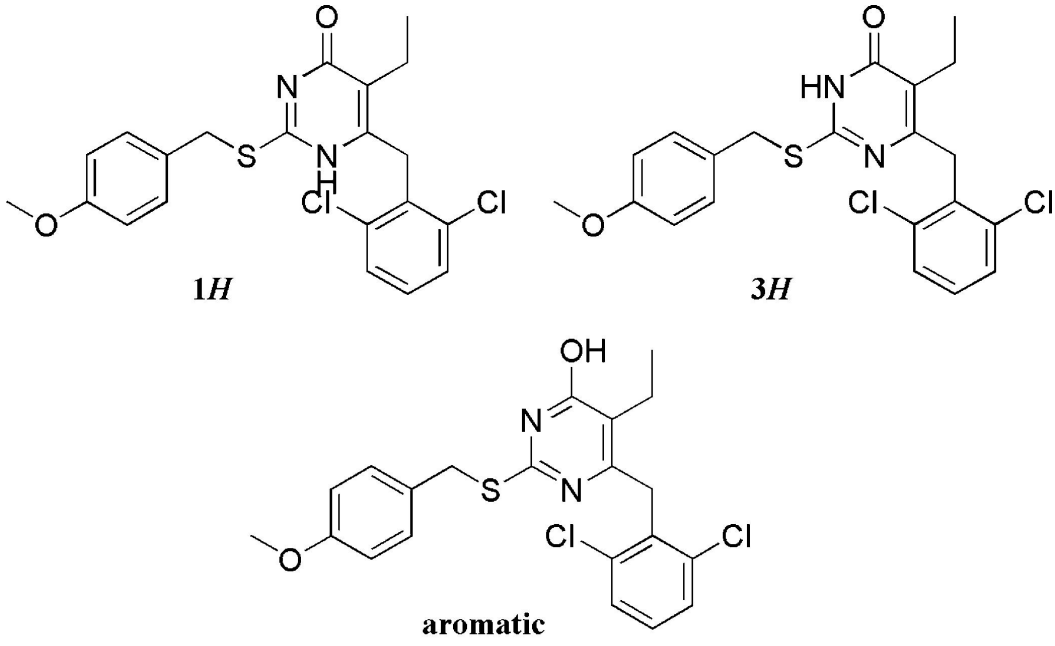
O1—C2—C7—C6	−179.0 (3)	C12—C15—C16—C17	−99.4 (4)
C5—C6—C7—C2	1.0 (6)	C12—C15—C16—C21	76.8 (4)
C4—C5—C8—S1	−92.8 (4)	C21—C16—C17—C18	0.4 (7)
C6—C5—C8—S1	86.6 (4)	C15—C16—C17—C18	176.8 (5)
C9—S1—C8—C5	−178.5 (3)	C21—C16—C17—Cl1	−178.6 (3)
C12—N2—C9—N1	−0.4 (5)	C15—C16—C17—Cl1	−2.2 (5)
C12—N2—C9—S1	179.8 (2)	C16—C17—C18—C19	−0.3 (13)
C10—N1—C9—N2	−2.2 (5)	Cl1—C17—C18—C19	178.6 (8)
C10—N1—C9—S1	177.7 (3)	C17—C18—C19—C20	2.2 (17)
C8—S1—C9—N2	−3.9 (4)	C18—C19—C20—C21	−4.1 (16)
C8—S1—C9—N1	176.2 (3)	C19—C20—C21—C16	4.0 (10)
C9—N1—C10—O2	−178.6 (3)	C19—C20—C21—Cl2	−176.6 (7)
C9—N1—C10—C11	2.3 (5)	C17—C16—C21—C20	−2.2 (6)
O2—C10—C11—C12	−179.1 (3)	C15—C16—C21—C20	−178.6 (4)
N1—C10—C11—C12	0.0 (5)	C17—C16—C21—Cl2	178.4 (3)
O2—C10—C11—C13	2.1 (5)	C15—C16—C21—Cl2	2.0 (5)
N1—C10—C11—C13	−178.8 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15B···Cl1	0.97	2.56	3.043 (4)	111
C7—H7···O1^{i}	0.93	2.49	3.389 (5)	162
N1—H1···O2^{ii}	0.858 (10)	1.921 (11)	2.777 (4)	175 (3)

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

Fig. 1



I

Fig. 2

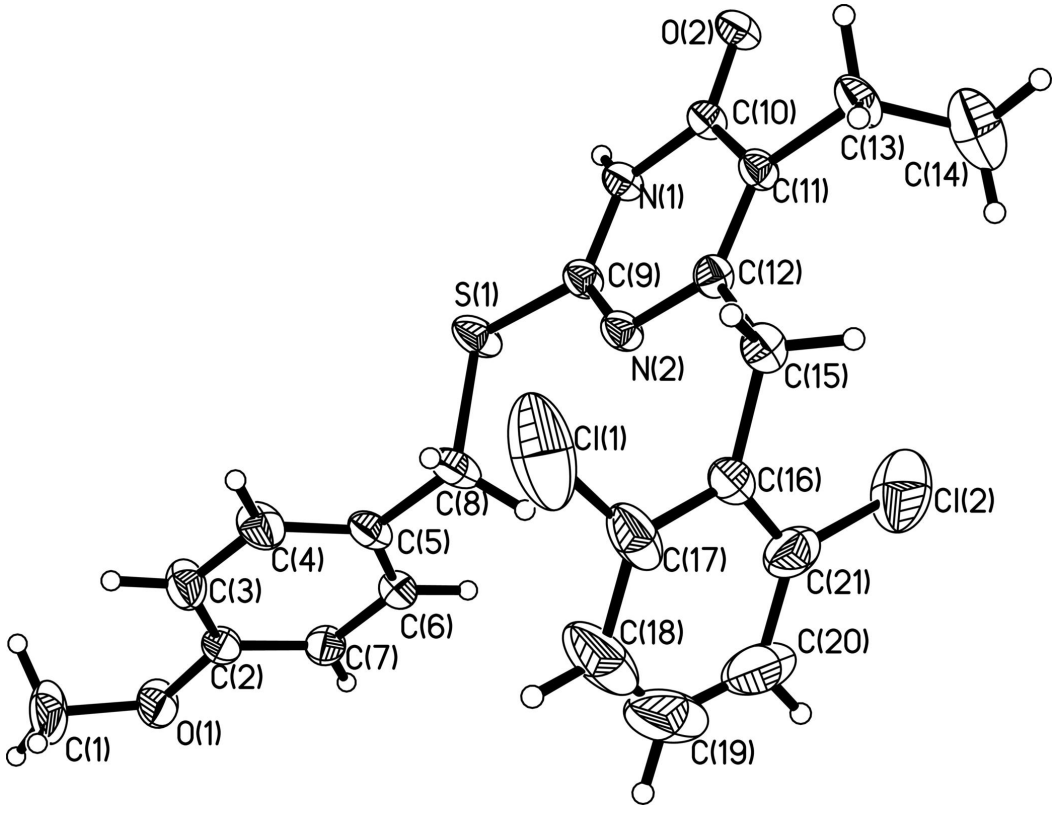

O(2)
C(10)
C(13)
C(14)
N(1)
C(11)
S(1)
C(9)
C(12)
N(2)
C(15)
Cl(1)
C(8)
C(16)
Cl(2)
C(4)
C(5)
C(17)
C(21)
C(3)
C(6)
C(18)
C(20)
C(7)
C(2)
O(1)
C(1)
C(19)

Fig. 3