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2-(Benzoylmethylsulfanyl)-6-benzyl-5-isopropylpyrimidin-4(3*H*)-one

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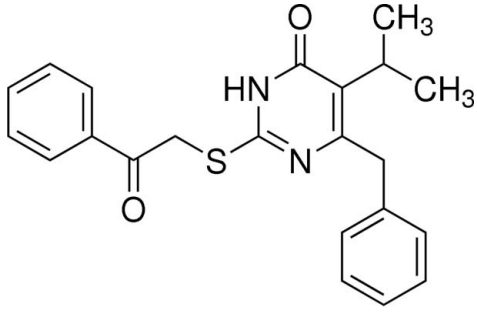
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.065; wR factor = 0.138; data-to-parameter ratio = 17.9.

The title compound, $C_{22}H_{22}N_2O_2S$, shows remarkable activity against HIV-1. The benzoyl and benzyl rings form dihedral angles of 85.7 (2) and 77.4 (3)°, respectively, with the pyrimidine ring. The dihedral angle between the two phenyl rings is 19.3 (3)°. Intramolecular C—H···N and C—H···O hydrogen bonds stabilize the molecular structure. Centrosymmetrically related molecules are linked by N—H···O hydrogen bonds into a dimer. In addition, intermolecular C—H···O hydrogen bonds are observed

Related literature

For related literature, see: He *et al.* (2004).



Experimental

Crystal data

$C_{22}H_{22}N_2O_2S$
M_r = 378.48
Monoclinic, $P2_1/n$
a = 8.691 (2) Å
b = 23.223 (6) Å
c = 10.705 (3) Å
β = 111.949 (4)°
V = 2004.1 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 298 (2) K
0.30 × 0.19 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.961, T_{max} = 0.987
12473 measured reflections
4358 independent reflections
1348 reflections with $I > 2\sigma(I)$
R_{int} = 0.103

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.138
S = 1.00
4358 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.86	1.89	2.747 (4)	177
C6—H6A···O1^{ii}	0.93	2.56	3.388 (5)	148
C8—H8A···N2	0.97	2.47	2.879 (5)	105
C14—H14C···O2	0.96	2.34	2.984 (5)	124

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

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: CI2429).

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  doi:10.1107/S1600536807037610

supplementary materials

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2-(Benzoylmethylsulfanyl)-6-benzyl-5-isopropylpyrimidin-4(3*H*)-one

Z.-K. Rao, S.-S. Zhang, Y.-P. He, Y.-T. Zheng and C. Li

Comment

As part of our ongoing investigation on the 2-arylcarbonylmethyl S-DABOs analogues (He *et al.*, 2004), the title compound was synthesized as a novel inhibitor, and it shows remarkable activity against HIV-1. Its molecular structure contains a pyrimidine and two phenyl rings (Fig. 1). The C1–C6 and C17–C22 phenyl rings form dihedral angles of 85.7 (2)° and 77.4 (3)°, respectively, with the pyrimidine ring. The dihedral angle between the two phenyl rings is 19.3 (3)°. The C17—C16—C12 bond angle between the pyrimidine and C17–C22 rings is 114.2 (3)°.

Intramolecular C—H···N and C—H···O type hydrogen bonds stabilize the molecular structure. The centrosymmetrically related molecules are linked by N—H···O hydrogen bonds into a dimer (Fig. 2). In addition, intermolecular C—H···O hydrogen bonds are observed (Table 1).

Experimental

The title compound was prepared according to the procedure of He *et al.* (2004). Single crystals were obtained from an ethyl acetate solution by slow evaporation at room temperature.

Refinement

Methyl H atoms were placed in calculated positions with C—H = 0.96 Å and torsion angle was refined to fit the electron density with U_{iso}(H) = 1.5U_{eq}(C). Other H were placed in calculated positions with C—H = 0.93–0.97 Å and N—H = 0.86 Å, and refined in riding mode, U_{iso}(H) = 1.2U_{eq}(C,*N*). Owing to the poor diffraction quality of the crystal, the ratio of observed to unique reflections is low (31%) and the R_{int} value is high (0.103).

Figures

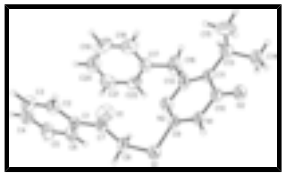

Fig. 1. The molecular structure of the title compound, showing the atom-labelling scheme and 30% probability displacement ellipsoids.

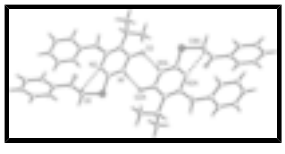

Fig. 2. A view of a N—H···O hydrogen-bonded dimer. Hydrogen bonds are shown as dashed lines. Atoms labelled with the suffix A are generated by the symmetry operation (1 − *x*, −*y*, 1 − *z*).

2-(Benzoylmethylsulfanyl)-6-benzyl-5-isopropylpyrimidin-4(3*H*)-one

Crystal data

$C_{22}H_{22}N_2O_2S$	$Z = 4$
$M_r = 378.48$	$F_{000} = 800$
Monoclinic, $P2_1/n$	$D_x = 1.254$ Mg m^{-3}
Hall symbol: -P 2yn	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.691$ (2) Å	$\theta = 1.8$–27.0º
$b = 23.223$ (6) Å	$\mu = 0.18$ mm^{-1}
$c = 10.705$ (3) Å	$T = 298$ (2) K
$\beta = 111.949$ (4)º	Plate, colourless
$V = 2004.1$ (9) Å^3	0.30 × 0.19 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer	4358 independent reflections
Radiation source: fine-focus sealed tube	1348 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.103$
$T = 298$(2) K	$\theta_{max} = 27.0$º
φ and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$h = -11 \rightarrow 11$
$T_{min} = 0.961$, $T_{max} = 0.987$	$k = -24 \rightarrow 29$
12473 measured reflections	$l = -11 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.065$	H-atom parameters constrained
$wR(F^2) = 0.138$	$w = 1/[\sigma^2(F_o^2) + (0.039P)^2]$ where $P = (F_o^2 + 2F_c^2)$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
4358 reflections	$\Delta\rho_{max} = 0.19$ e Å^{-3}
244 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. 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 calculat-

ing *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.

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}
S1	0.74405 (15)	0.14324 (5)	0.58050 (11)	0.0803 (4)
O1	0.5071 (3)	0.23901 (12)	0.4777 (3)	0.0893 (10)
O2	0.3701 (3)	−0.00995 (11)	0.5886 (2)	0.0705 (8)
N1	0.5429 (4)	0.06432 (13)	0.6032 (3)	0.0591 (9)
H1A	0.5734	0.0479	0.5442	0.071*
N2	0.5769 (4)	0.14324 (13)	0.7453 (3)	0.0720 (10)
C1	0.6581 (5)	0.31823 (17)	0.5976 (4)	0.0521 (10)
C2	0.5386 (5)	0.3564 (2)	0.5210 (4)	0.0753 (13)
H2B	0.4443	0.3426	0.4523	0.090*
C3	0.5575 (6)	0.4147 (2)	0.5452 (5)	0.0975 (16)
H3A	0.4763	0.4401	0.4927	0.117*
C4	0.6947 (7)	0.4352 (2)	0.6456 (6)	0.1010 (17)
H4A	0.7071	0.4746	0.6611	0.121*
C5	0.8153 (6)	0.3981 (2)	0.7244 (4)	0.0914 (15)
H5A	0.9089	0.4122	0.7934	0.110*
C6	0.7952 (5)	0.33933 (19)	0.6994 (4)	0.0718 (12)
H6A	0.8760	0.3140	0.7525	0.086*
C7	0.6320 (5)	0.25571 (18)	0.5645 (4)	0.0577 (11)
C8	0.7706 (5)	0.21571 (14)	0.6419 (4)	0.0666 (12)
H8A	0.7811	0.2154	0.7353	0.080*
H8B	0.8735	0.2307	0.6391	0.080*
C9	0.6094 (5)	0.11632 (16)	0.6528 (4)	0.0594 (11)
C10	0.4286 (5)	0.03664 (18)	0.6432 (4)	0.0588 (11)
C11	0.3910 (5)	0.06488 (17)	0.7479 (4)	0.0591 (11)
C12	0.4662 (6)	0.11664 (18)	0.7929 (4)	0.0717 (13)
C13	0.2691 (5)	0.03583 (18)	0.7980 (4)	0.0761 (13)
H13A	0.2676	0.0580	0.8754	0.091*
C14	0.3136 (5)	−0.02547 (18)	0.8449 (4)	0.0980 (15)
H14A	0.2296	−0.0413	0.8728	0.147*
H14B	0.4184	−0.0260	0.9193	0.147*
H14C	0.3212	−0.0481	0.7723	0.147*
C15	0.0966 (6)	0.0379 (2)	0.6919 (5)	0.143 (2)
H15A	0.0693	0.0769	0.6621	0.215*
H15B	0.0188	0.0238	0.7289	0.215*
H15C	0.0916	0.0143	0.6169	0.215*
C16	0.4398 (6)	0.15025 (17)	0.9048 (4)	0.1119 (18)
H16A	0.3314	0.1407	0.9053	0.134*

H16B	0.5221	0.1381	0.9904	0.134*
C17	0.4508 (7)	0.21374 (19)	0.8932 (5)	0.0658 (12)
C18	0.3165 (7)	0.2464 (3)	0.8216 (5)	0.0944 (16)
H18A	0.2148	0.2283	0.7786	0.113*
C19	0.3263 (9)	0.3049 (4)	0.8110 (6)	0.118 (2)
H19A	0.2322	0.3262	0.7624	0.142*
C20	0.4709 (11)	0.3311 (3)	0.8706 (7)	0.112 (2)
H20A	0.4779	0.3707	0.8610	0.135*
C21	0.6078 (7)	0.3015 (3)	0.9445 (6)	0.1028 (18)
H21A	0.7078	0.3205	0.9880	0.123*
C22	0.5972 (7)	0.2424 (3)	0.9547 (4)	0.0835 (14)
H22A	0.6919	0.2217	1.0046	0.100*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.1087 (9)	0.0565 (8)	0.1015 (9)	−0.0011 (7)	0.0689 (8)	−0.0034 (7)
O1	0.070 (2)	0.086 (2)	0.088 (2)	−0.0099 (18)	0.0023 (17)	−0.0288 (18)
O2	0.094 (2)	0.0537 (19)	0.079 (2)	−0.0062 (16)	0.0503 (17)	−0.0155 (15)
N1	0.086 (2)	0.045 (2)	0.060 (2)	0.0038 (19)	0.0430 (19)	−0.0075 (18)
N2	0.115 (3)	0.051 (2)	0.072 (2)	−0.011 (2)	0.061 (2)	−0.0165 (19)
C1	0.057 (3)	0.051 (3)	0.051 (3)	0.005 (2)	0.023 (2)	0.008 (2)
C2	0.085 (3)	0.071 (3)	0.073 (3)	−0.003 (3)	0.032 (3)	−0.004 (3)
C3	0.098 (4)	0.085 (5)	0.108 (4)	0.021 (4)	0.036 (3)	0.017 (3)
C4	0.137 (6)	0.058 (4)	0.127 (5)	0.001 (4)	0.071 (4)	0.002 (4)
C5	0.109 (4)	0.071 (4)	0.087 (4)	−0.032 (3)	0.029 (3)	−0.018 (3)
C6	0.081 (3)	0.065 (3)	0.064 (3)	−0.014 (3)	0.022 (3)	−0.003 (2)
C7	0.064 (3)	0.058 (3)	0.054 (3)	−0.005 (3)	0.026 (2)	−0.002 (2)
C8	0.081 (3)	0.052 (3)	0.069 (3)	−0.005 (2)	0.030 (2)	0.000 (2)
C9	0.082 (3)	0.045 (3)	0.062 (3)	0.007 (2)	0.039 (2)	0.003 (2)
C10	0.071 (3)	0.052 (3)	0.061 (3)	0.006 (3)	0.033 (2)	0.004 (2)
C11	0.084 (3)	0.049 (3)	0.059 (3)	0.004 (2)	0.043 (2)	−0.004 (2)
C12	0.121 (4)	0.048 (3)	0.067 (3)	0.008 (3)	0.058 (3)	−0.001 (2)
C13	0.103 (4)	0.063 (3)	0.090 (3)	0.002 (3)	0.068 (3)	−0.009 (3)
C14	0.129 (4)	0.076 (4)	0.107 (4)	−0.016 (3)	0.065 (3)	0.011 (3)
C15	0.078 (4)	0.191 (6)	0.177 (5)	0.037 (4)	0.068 (4)	0.058 (5)
C16	0.220 (6)	0.054 (3)	0.107 (4)	−0.017 (4)	0.112 (4)	−0.029 (3)
C17	0.096 (4)	0.057 (3)	0.064 (3)	−0.002 (3)	0.053 (3)	−0.016 (3)
C18	0.095 (4)	0.113 (5)	0.072 (4)	0.007 (4)	0.027 (3)	−0.022 (4)
C19	0.128 (6)	0.142 (7)	0.089 (4)	0.068 (5)	0.045 (4)	0.021 (5)
C20	0.175 (7)	0.079 (5)	0.121 (6)	0.024 (5)	0.098 (6)	0.004 (4)
C21	0.101 (5)	0.104 (5)	0.121 (5)	−0.031 (4)	0.061 (4)	−0.047 (4)
C22	0.089 (4)	0.084 (4)	0.078 (3)	0.019 (3)	0.033 (3)	−0.011 (3)

Geometric parameters (Å, °)

S1—C9	1.743 (4)	C11—C13	1.514 (5)
S1—C8	1.790 (3)	C12—C16	1.518 (5)
O1—C7	1.199 (4)	C13—C15	1.506 (5)

O2—C10	1.244 (4)	C13—C14	1.511 (5)
N1—C9	1.358 (4)	C13—H13A	0.98
N1—C10	1.379 (4)	C14—H14A	0.96
N1—H1A	0.86	C14—H14B	0.96
N2—C9	1.288 (4)	C14—H14C	0.96
N2—C12	1.391 (4)	C15—H15A	0.96
C1—C6	1.370 (5)	C15—H15B	0.96
C1—C2	1.379 (5)	C15—H15C	0.96
C1—C7	1.491 (5)	C16—C17	1.486 (5)
C2—C3	1.376 (5)	C16—H16A	0.97
C2—H2B	0.93	C16—H16B	0.97
C3—C4	1.358 (5)	C17—C18	1.362 (6)
C3—H3A	0.93	C17—C22	1.367 (5)
C4—C5	1.376 (5)	C18—C19	1.370 (7)
C4—H4A	0.93	C18—H18A	0.93
C5—C6	1.389 (5)	C19—C20	1.325 (7)
C5—H5A	0.93	C19—H19A	0.93
C6—H6A	0.93	C20—C21	1.344 (6)
C7—C8	1.502 (5)	C20—H20A	0.93
C8—H8A	0.97	C21—C22	1.383 (6)
C8—H8B	0.97	C21—H21A	0.93
C10—C11	1.438 (4)	C22—H22A	0.93
C11—C12	1.367 (5)		
C9—S1—C8	100.97 (18)	N2—C12—C16	113.0 (4)
C9—N1—C10	122.9 (3)	C15—C13—C14	109.9 (4)
C9—N1—H1A	118.5	C15—C13—C11	110.5 (4)
C10—N1—H1A	118.5	C14—C13—C11	114.3 (3)
C9—N2—C12	116.5 (3)	C15—C13—H13A	107.3
C6—C1—C2	118.8 (4)	C14—C13—H13A	107.3
C6—C1—C7	123.2 (4)	C11—C13—H13A	107.3
C2—C1—C7	118.1 (4)	C13—C14—H14A	109.5
C3—C2—C1	120.7 (4)	C13—C14—H14B	109.5
C3—C2—H2B	119.7	H14A—C14—H14B	109.5
C1—C2—H2B	119.7	C13—C14—H14C	109.5
C4—C3—C2	120.1 (5)	H14A—C14—H14C	109.5
C4—C3—H3A	119.9	H14B—C14—H14C	109.5
C2—C3—H3A	119.9	C13—C15—H15A	109.5
C3—C4—C5	120.5 (5)	C13—C15—H15B	109.5
C3—C4—H4A	119.7	H15A—C15—H15B	109.5
C5—C4—H4A	119.7	C13—C15—H15C	109.5
C4—C5—C6	119.0 (4)	H15A—C15—H15C	109.5
C4—C5—H5A	120.5	H15B—C15—H15C	109.5
C6—C5—H5A	120.5	C17—C16—C12	114.2 (3)
C1—C6—C5	120.9 (4)	C17—C16—H16A	108.7
C1—C6—H6A	119.5	C12—C16—H16A	108.7
C5—C6—H6A	119.5	C17—C16—H16B	108.7
O1—C7—C1	120.8 (4)	C12—C16—H16B	108.7
O1—C7—C8	122.3 (4)	H16A—C16—H16B	107.6
C1—C7—C8	116.8 (4)	C18—C17—C22	116.6 (4)

C7—C8—S1	114.4 (3)	C18—C17—C16	122.1 (6)
C7—C8—H8A	108.7	C22—C17—C16	121.3 (5)
S1—C8—H8A	108.7	C17—C18—C19	122.1 (6)
C7—C8—H8B	108.7	C17—C18—H18A	118.9
S1—C8—H8B	108.7	C19—C18—H18A	118.9
H8A—C8—H8B	107.6	C20—C19—C18	119.5 (7)
N2—C9—N1	123.3 (3)	C20—C19—H19A	120.3
N2—C9—S1	122.9 (3)	C18—C19—H19A	120.3
N1—C9—S1	113.8 (3)	C19—C20—C21	121.4 (7)
O2—C10—N1	118.4 (4)	C19—C20—H20A	119.3
O2—C10—C11	126.2 (4)	C21—C20—H20A	119.3
N1—C10—C11	115.4 (4)	C20—C21—C22	118.9 (6)
C12—C11—C10	117.2 (4)	C20—C21—H21A	120.6
C12—C11—C13	124.9 (4)	C22—C21—H21A	120.6
C10—C11—C13	117.8 (4)	C17—C22—C21	121.5 (5)
C11—C12—N2	124.5 (3)	C17—C22—H22A	119.3
C11—C12—C16	122.5 (4)	C21—C22—H22A	119.3

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O2^{i}	0.86	1.89	2.747 (4)	177
C6—H6A···O1^{ii}	0.93	2.56	3.388 (5)	148
C8—H8A···N2	0.97	2.47	2.879 (5)	105
C14—H14C···O2	0.96	2.34	2.984 (5)	124

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

Fig. 1

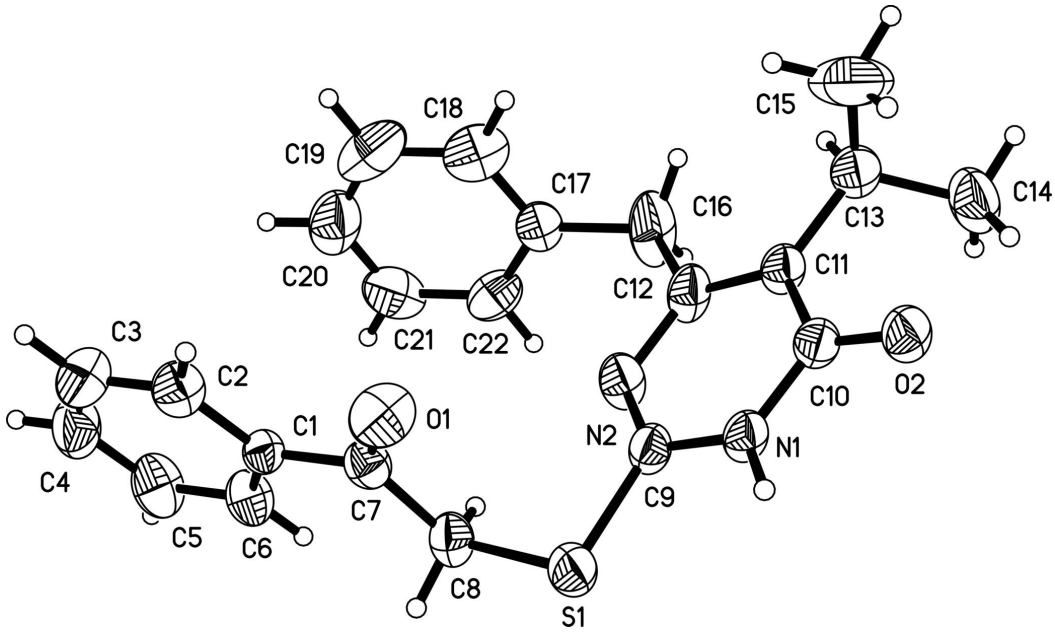
C18
C15
C19
C17
C16
C13
C14
C20
C12
C11
C3
C21
C22
C2
O1
C10
O2
C1
N2
N1
C4
C7
C9
C5
C6
C8
S1

Fig. 2