Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 1-butyl-6-methyl-2-phenyl-4-thioxo-1,4-dihydropyrimidine-5-carboxylate[1]

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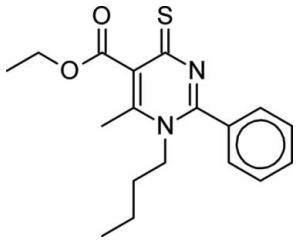
Received 2 April 2007; accepted 21 April 2007

Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.052; wR factor = 0.135; data-to-parameter ratio = 9.5.

The title compound, $C_{18}H_{22}N_2O_2S$, is of interest with respect to antibacterial and anticancer activity and it has shown good trypanocidal activity. The molecular packing lacks classical hydrogen bonds, being mediated only by weak van der Waals forces.

Related literature

For the synthesis, see: Cunha *et al.* (2007). A butyl group on atom N1 in this structure replaces a hydroxyethyl group in the derivatives described in the preceding papers (Sabino, Lariucci *et al.*, 2007; Sabino, Vencato *et al.*, 2007). Owing to the different chemical nature of the butyl group, the title compound does not pack in the same manner and lacks the intermolecular hydrogen-bond contacts observed in the previous derivatives.



Experimental

Crystal data

$C_{18}H_{22}N_2O_2S$
M_r = 330.45
Monoclinic, $P2_1$
a = 10.9870 (18) Å
b = 7.2840 (14) Å
c = 12.5885 (13) Å
β = 115.591 (9)°
V = 908.6 (3) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 1.66 mm^{-1}
T = 297 (2) K
0.35 × 0.25 × 0.05 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.594, T_{max} = 0.922
2129 measured reflections
2034 independent reflections
1907 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
2 standard reflections
frequency: 120 min
intensity decay: 2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.136
S = 1.09
2034 reflections
214 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}
Absolute structure: Flack (1983), 270 Friedel pairs
Flack parameter: 0.10 (3)

Data collection: *CAD-4-PC* (Enraf–Nonius, 1993); cell refinement: *CAD-4-PC*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors gratefully acknowledge the financial support of Conselho Nacional de Desenvolvimento Científico e Tecnológico – CNPq and Fundação de Amparo à Pesquisa do Estado da Bahia – FAPESB. We also thank CNPq for a research fellowship to SC and IV.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2100).

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[1] Structural studies of 4-thioxopyrimidines. Part 3.

  doi:10.1107/S1600536807019964

supplementary materials

Acta Cryst. (2007). E**63**, o2852 [**doi:10.1107/S1600536807019964**]

Ethyl 1-butyl-6-methyl-2-phenyl-4-thioxo-1,4-dihydropyrimidine-5-carboxylate

J. R. Sabino, I. Vencato, R. M. Bastos and S. Cunha

Comment

In continuation of our solid-state studies of bioactive thioxopyrimidine, we performed the crystallographic characterization of the title 4-thioxopyrimidine (I), which exhibited a lowered antifungal but enhanced trypanocidal activities compared to related compounds (Cunha *et al.*, 2007).

The molecule of (I) is depicted in Fig. 1. This derivative differs from those of Parts 1 and 2 by a substituent on the ring atom N1, where (I) has a butyl group instead of a hydroxyethyl group. The conformation of compound (I) is defined by steric effects. The pyrimidine ring is planar with an r.m.s. deviation of 0.022 Å. With reference to this plane, the phenyl ring is rotated by 65.0 (1)°, approaching a *gauche* conformation. The torsion angles C4—C5—C14—O15 and C20—C19—N1—C6 are -99.3 (4)° and -92.9 (3)°, respectively. Bond lengths are within the expected ranges with the exception of the C2–C7 and C5–C14 bonds which are elongated by an average of 0.035 Å from the formal single bond distance.

It is interesting to note that the crystal packing of compound (I) is maintained by van der Waals forces only; it does not form dimers involving C═O···π-ring interactions as observed in the previous derivatives. It is supposed that the steric inaccessibility due to the long butyl substituent group prevents the pyrimidine ring stacking. The packing is shown in Fig. 2.

Experimental

Compound (I) (m.p. 447.6–448.6 K) was prepared according to a known procedure (Cunha *et al.*, 2007). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a solution in $CHCl_3$ at room temperature.

Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $U_{iso}(H) = 1.2U_{eq}(C)$ for other atoms. The C18 methyl atom were modelled as a disordered group over two sites with refined occupancies 0.80 (2) and 0.20 (2), and refined with equal displacement parameter constraints. In consequence, the bond length C17–C18 was poorly determined. The whole carboxylate group is possibly disordered by a rotation around the C5–C14 σ-bond, but this could not be modelled reliably.

Figures

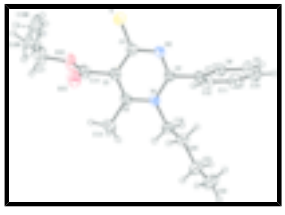

Fig. 1. The molecular structure of (I) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius.

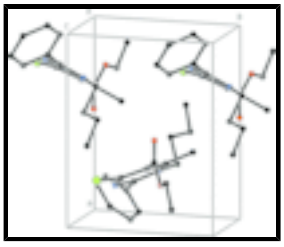

Fig. 2. Packing diagram of (I).

Ethyl 1-butyl-6-methyl-2-phenyl-4-thioxo-1,4-dihydropyrimidine-5-carboxylate

Crystal data

$C_{18}H_{22}N_2O_2S$	F_{000} = 352
M_r = 330.45	D_x = 1.208 Mg m^{-3}
Monoclinic, $P2_1$	Cu $K\alpha$ radiation λ = 1.54180 Å
Hall symbol: P 2yb	Cell parameters from 25 reflections
a = 10.9870 (18) Å	θ = 12.9–40.6º
b = 7.2840 (14) Å	μ = 1.66 mm^{-1}
c = 12.5885 (13) Å	T = 297 (2) K
β = 115.591 (9)º	Prism, yellow
V = 908.6 (3) Å^3	0.35 × 0.25 × 0.05 mm
Z = 2	

Data collection

Enraf–Nonius CAD-4 diffractometer	θ_{max} = 67.1º
T = 297(2) K	θ_{min} = 3.9º
ω/2θ scans	h = −13→11
Absorption correction: ψ scan (North *et al.*, 1968)	k = −1→8
T_{min} = 0.594, T_{max} = 0.922	l = 0→15
2129 measured reflections	2 standard reflections
2034 independent reflections	every 120 min
1907 reflections with $I > 2\sigma(I)$	intensity decay: 2%
R_{int} = 0.047	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1111P)^2 + 0.0314P]$ where $P = (F_o^2 + 2F_c^2)/3$
Least-squares matrix: full	$(\Delta/\sigma)_{max} < 0.001$
$R[F^2 > 2\sigma(F^2)]$ = 0.052	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$wR(F^2)$ = 0.136	$\Delta\rho_{min}$ = −0.44 e Å^{-3}
S = 1.09	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

2034 reflections
214 parameters
1 restraint
H-atom parameters constrained

Extinction coefficient: 0.034 (3)
Absolute structure: Flack (1983), 270 Friedel pairs
Flack parameter: 0.10 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S	0.77081 (9)	0.15710 (13)	0.75355 (7)	0.0651 (3)	
N1	0.7310 (2)	0.5282 (3)	0.46126 (19)	0.0458 (5)	
C2	0.7929 (2)	0.3596 (4)	0.4803 (2)	0.0423 (6)	
N3	0.8080 (2)	0.2499 (4)	0.5663 (2)	0.0466 (5)	
C4	0.7614 (3)	0.3022 (4)	0.6479 (2)	0.0463 (6)	
C5	0.7055 (2)	0.4821 (4)	0.6357 (2)	0.0462 (6)	
C6	0.6850 (3)	0.5898 (4)	0.5420 (2)	0.0476 (6)	
C7	0.8475 (2)	0.2935 (4)	0.3973 (2)	0.0435 (6)	
C8	0.7920 (3)	0.1380 (5)	0.3314 (2)	0.0508 (7)	
H8	0.7191	0.0806	0.3365	0.061*	
C9	0.8442 (3)	0.0673 (6)	0.2581 (3)	0.0632 (8)	
H9	0.8066	−0.0378	0.2142	0.076*	
C10	0.9521 (3)	0.1521 (7)	0.2496 (3)	0.0665 (9)	
H10	0.9874	0.1041	0.2002	0.08*	
C11	1.0069 (3)	0.3070 (7)	0.3139 (3)	0.0681 (10)	
H11	1.0784	0.3652	0.3069	0.082*	
C12	0.9574 (3)	0.3781 (5)	0.3895 (3)	0.0575 (8)	
H12	0.997	0.4814	0.4346	0.069*	
C13	0.6183 (4)	0.7740 (6)	0.5228 (3)	0.0734 (10)	
H13A	0.542	0.7765	0.4471	0.11*	
H13B	0.6814	0.8674	0.5259	0.11*	
H13C	0.5888	0.7963	0.5832	0.11*	
C14	0.6638 (3)	0.5473 (5)	0.7281 (3)	0.0556 (7)	
O15	0.5505 (2)	0.5468 (6)	0.7192 (2)	0.0825 (9)	
O16	0.7694 (2)	0.6091 (5)	0.82076 (18)	0.0664 (7)	
C17	0.7489 (5)	0.6655 (11)	0.9216 (4)	0.1002 (18)	
H17A	0.6863	0.7678	0.9003	0.12*	
H17B	0.7103	0.565	0.9474	0.12*	
C18A	0.8742 (8)	0.719 (3)	1.0149 (7)	0.154 (6)	0.807 (19)
H18A	0.8707	0.7003	1.089	0.231*	0.807 (19)
H18B	0.8908	0.8461	1.0063	0.231*	0.807 (19)
H18C	0.9455	0.6458	1.0122	0.231*	0.807 (19)
C18B	0.843 (4)	0.569 (11)	1.019 (3)	0.154 (6)	0.193 (19)
H18D	0.8499	0.625	1.0903	0.231*	0.193 (19)

H18E	0.93	0.573	1.0174	0.231*	0.193 (19)
H18F	0.815	0.4439	1.0157	0.231*	0.193 (19)
C19	0.7021 (3)	0.6331 (5)	0.3526 (2)	0.0546 (7)	
H19A	0.778	0.6213	0.3329	0.066*	
H19B	0.6928	0.762	0.367	0.066*	
C20	0.5751 (3)	0.5694 (5)	0.2488 (2)	0.0565 (7)	
H20A	0.4982	0.5836	0.2668	0.068*	
H20B	0.5832	0.4404	0.2338	0.068*	
C21	0.5532 (4)	0.6817 (7)	0.1401 (2)	0.0729 (10)	
H21A	0.55	0.8108	0.1576	0.087*	
H21B	0.6297	0.6638	0.1219	0.087*	
C22	0.4257 (5)	0.6321 (9)	0.0332 (3)	0.0909 (13)	
H22A	0.4174	0.7079	−0.032	0.136*	
H22B	0.3493	0.6514	0.0499	0.136*	
H22C	0.4293	0.5054	0.0137	0.136*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S	0.0847 (5)	0.0628 (5)	0.0606 (4)	0.0110 (4)	0.0435 (4)	0.0122 (4)
N1	0.0506 (11)	0.0397 (12)	0.0433 (11)	0.0013 (10)	0.0166 (9)	−0.0012 (10)
C2	0.0426 (11)	0.0394 (14)	0.0428 (12)	−0.0002 (10)	0.0163 (10)	−0.0022 (11)
N3	0.0534 (11)	0.0428 (13)	0.0476 (11)	0.0064 (11)	0.0255 (9)	0.0035 (11)
C4	0.0426 (12)	0.0493 (15)	0.0463 (13)	−0.0003 (12)	0.0186 (10)	−0.0024 (13)
C5	0.0388 (11)	0.0492 (16)	0.0475 (13)	−0.0005 (11)	0.0157 (9)	−0.0088 (12)
C6	0.0448 (12)	0.0441 (14)	0.0470 (13)	0.0032 (11)	0.0134 (10)	−0.0076 (12)
C7	0.0437 (12)	0.0437 (14)	0.0441 (12)	0.0013 (11)	0.0200 (9)	0.0026 (12)
C8	0.0529 (13)	0.0488 (17)	0.0592 (14)	−0.0056 (13)	0.0322 (11)	−0.0033 (14)
C9	0.0650 (16)	0.070 (2)	0.0627 (17)	−0.0080 (16)	0.0350 (14)	−0.0179 (18)
C10	0.0630 (16)	0.087 (3)	0.0629 (16)	0.008 (2)	0.0401 (13)	0.002 (2)
C11	0.0493 (14)	0.088 (3)	0.078 (2)	−0.0044 (17)	0.0380 (14)	0.005 (2)
C12	0.0467 (13)	0.0606 (18)	0.0642 (17)	−0.0108 (13)	0.0230 (12)	−0.0040 (16)
C13	0.086 (2)	0.057 (2)	0.068 (2)	0.026 (2)	0.0248 (17)	−0.0021 (18)
C14	0.0483 (13)	0.0607 (19)	0.0589 (15)	0.0017 (14)	0.0243 (11)	−0.0098 (15)
O15	0.0518 (11)	0.118 (3)	0.0857 (15)	0.0043 (14)	0.0368 (10)	−0.0215 (18)
O16	0.0597 (11)	0.0851 (18)	0.0565 (11)	−0.0044 (12)	0.0269 (9)	−0.0261 (12)
C17	0.096 (3)	0.136 (5)	0.077 (2)	−0.001 (3)	0.044 (2)	−0.045 (3)
C18A	0.100 (5)	0.269 (19)	0.080 (3)	−0.018 (7)	0.027 (3)	−0.099 (8)
C18B	0.100 (5)	0.269 (19)	0.080 (3)	−0.018 (7)	0.027 (3)	−0.099 (8)
C19	0.0628 (15)	0.0433 (16)	0.0532 (14)	0.0017 (13)	0.0208 (12)	0.0074 (14)
C20	0.0618 (15)	0.0568 (18)	0.0475 (14)	0.0066 (15)	0.0204 (11)	0.0068 (15)
C21	0.085 (2)	0.080 (3)	0.0484 (15)	−0.003 (2)	0.0241 (14)	0.0064 (18)
C22	0.109 (3)	0.093 (3)	0.0504 (16)	−0.009 (3)	0.0157 (17)	0.003 (2)

Geometric parameters (Å, °)

S—C4	1.666 (3)	C14—O15	1.201 (3)
N1—C2	1.374 (4)	C14—O16	1.319 (4)
N1—C6	1.390 (4)	O16—C17	1.442 (4)

N1—C19	1.477 (4)	C17—C18B	1.40 (6)
C2—N3	1.297 (4)	C17—C18A	1.424 (10)
C2—C7	1.492 (4)	C17—H17A	0.97
N3—C4	1.385 (3)	C17—H17B	0.97
C4—C5	1.427 (4)	C18A—H18A	0.96
C5—C6	1.353 (4)	C18A—H18B	0.96
C5—C14	1.499 (4)	C18A—H18C	0.96
C6—C13	1.498 (5)	C18B—H18D	0.96
C7—C8	1.381 (4)	C18B—H18E	0.96
C7—C12	1.396 (4)	C18B—H18F	0.96
C8—C9	1.380 (4)	C19—C20	1.515 (4)
C8—H8	0.93	C19—H19A	0.97
C9—C10	1.382 (5)	C19—H19B	0.97
C9—H9	0.93	C20—C21	1.522 (4)
C10—C11	1.367 (7)	C20—H20A	0.97
C10—H10	0.93	C20—H20B	0.97
C11—C12	1.384 (5)	C21—C22	1.508 (5)
C11—H11	0.93	C21—H21A	0.97
C12—H12	0.93	C21—H21B	0.97
C13—H13A	0.96	C22—H22A	0.96
C13—H13B	0.96	C22—H22B	0.96
C13—H13C	0.96	C22—H22C	0.96
C2—N1—C6	118.0 (2)	C18B—C17—O16	106.8 (16)
C2—N1—C19	121.1 (2)	C18A—C17—O16	109.9 (4)
C6—N1—C19	120.6 (2)	C18B—C17—H17A	142.5
N3—C2—N1	124.9 (2)	C18A—C17—H17A	109.7
N3—C2—C7	116.1 (2)	O16—C17—H17A	109.7
N1—C2—C7	119.0 (2)	C18B—C17—H17B	66.2
C2—N3—C4	119.7 (2)	C18A—C17—H17B	109.7
N3—C4—C5	116.9 (3)	O16—C17—H17B	109.7
N3—C4—S	120.2 (2)	H17A—C17—H17B	108.2
C5—C4—S	122.9 (2)	C17—C18A—H18A	109.5
C6—C5—C4	121.9 (2)	C17—C18A—H18B	109.5
C6—C5—C14	120.1 (3)	H18A—C18A—H18B	109.5
C4—C5—C14	118.0 (3)	C17—C18A—H18C	109.5
C5—C6—N1	118.3 (3)	H18A—C18A—H18C	109.5
C5—C6—C13	123.1 (3)	H18B—C18A—H18C	109.5
N1—C6—C13	118.6 (3)	C17—C18B—H18D	109.5
C8—C7—C12	119.4 (3)	C17—C18B—H18E	109.5
C8—C7—C2	118.6 (2)	H18D—C18B—H18E	109.5
C12—C7—C2	121.9 (3)	C17—C18B—H18F	109.5
C9—C8—C7	120.3 (3)	H18D—C18B—H18F	109.5
C9—C8—H8	119.8	H18E—C18B—H18F	109.5
C7—C8—H8	119.8	N1—C19—C20	112.9 (3)
C8—C9—C10	120.2 (4)	N1—C19—H19A	109
C8—C9—H9	119.9	C20—C19—H19A	109
C10—C9—H9	119.9	N1—C19—H19B	109
C11—C10—C9	119.7 (3)	C20—C19—H19B	109
C11—C10—H10	120.1	H19A—C19—H19B	107.8

C9—C10—H10	120.1	C19—C20—C21	109.8 (3)
C10—C11—C12	120.9 (3)	C19—C20—H20A	109.7
C10—C11—H11	119.6	C21—C20—H20A	109.7
C12—C11—H11	119.6	C19—C20—H20B	109.7
C11—C12—C7	119.4 (3)	C21—C20—H20B	109.7
C11—C12—H12	120.3	H20A—C20—H20B	108.2
C7—C12—H12	120.3	C22—C21—C20	113.5 (4)
C6—C13—H13A	109.5	C22—C21—H21A	108.9
C6—C13—H13B	109.5	C20—C21—H21A	108.9
H13A—C13—H13B	109.5	C22—C21—H21B	108.9
C6—C13—H13C	109.5	C20—C21—H21B	108.9
H13A—C13—H13C	109.5	H21A—C21—H21B	107.7
H13B—C13—H13C	109.5	C21—C22—H22A	109.5
O15—C14—O16	124.3 (3)	C21—C22—H22B	109.5
O15—C14—C5	125.3 (3)	H22A—C22—H22B	109.5
O16—C14—C5	110.3 (2)	C21—C22—H22C	109.5
C14—O16—C17	117.6 (3)	H22A—C22—H22C	109.5
C18B—C17—C18A	48 (3)	H22B—C22—H22C	109.5
C6—N1—C2—N3	2.4 (4)	N3—C2—C7—C12	−112.8 (3)
C19—N1—C2—N3	−171.8 (3)	N1—C2—C7—C12	67.4 (4)
C6—N1—C2—C7	−177.8 (2)	C12—C7—C8—C9	−0.3 (5)
C19—N1—C2—C7	8.0 (3)	C2—C7—C8—C9	−176.8 (3)
N1—C2—N3—C4	−0.9 (4)	C7—C8—C9—C10	−0.3 (5)
C7—C2—N3—C4	179.3 (2)	C8—C9—C10—C11	−0.2 (6)
C2—N3—C4—C5	−3.6 (3)	C9—C10—C11—C12	1.3 (6)
C2—N3—C4—S	175.89 (19)	C10—C11—C12—C7	−1.9 (6)
N3—C4—C5—C6	7.1 (4)	C8—C7—C12—C11	1.4 (5)
S—C4—C5—C6	−172.4 (2)	C2—C7—C12—C11	177.7 (3)
N3—C4—C5—C14	−175.5 (2)	C6—C5—C14—O15	78.1 (5)
S—C4—C5—C14	5.0 (3)	C4—C5—C14—O15	−99.3 (4)
C4—C5—C6—N1	−5.7 (4)	C6—C5—C14—O16	−100.7 (3)
C14—C5—C6—N1	176.9 (2)	C4—C5—C14—O16	81.8 (4)
C4—C5—C6—C13	175.9 (3)	O15—C14—O16—C17	5.4 (7)
C14—C5—C6—C13	−1.5 (4)	C5—C14—O16—C17	−175.8 (4)
C2—N1—C6—C5	1.0 (4)	C14—O16—C17—C18B	126 (3)
C19—N1—C6—C5	175.2 (2)	C14—O16—C17—C18A	177.0 (9)
C2—N1—C6—C13	179.5 (3)	C2—N1—C19—C20	81.1 (3)
C19—N1—C6—C13	−6.3 (4)	C6—N1—C19—C20	−92.9 (3)
N3—C2—C7—C8	63.6 (3)	N1—C19—C20—C21	−179.2 (3)
N1—C2—C7—C8	−116.2 (3)	C19—C20—C21—C22	−177.8 (4)

Fig. 1

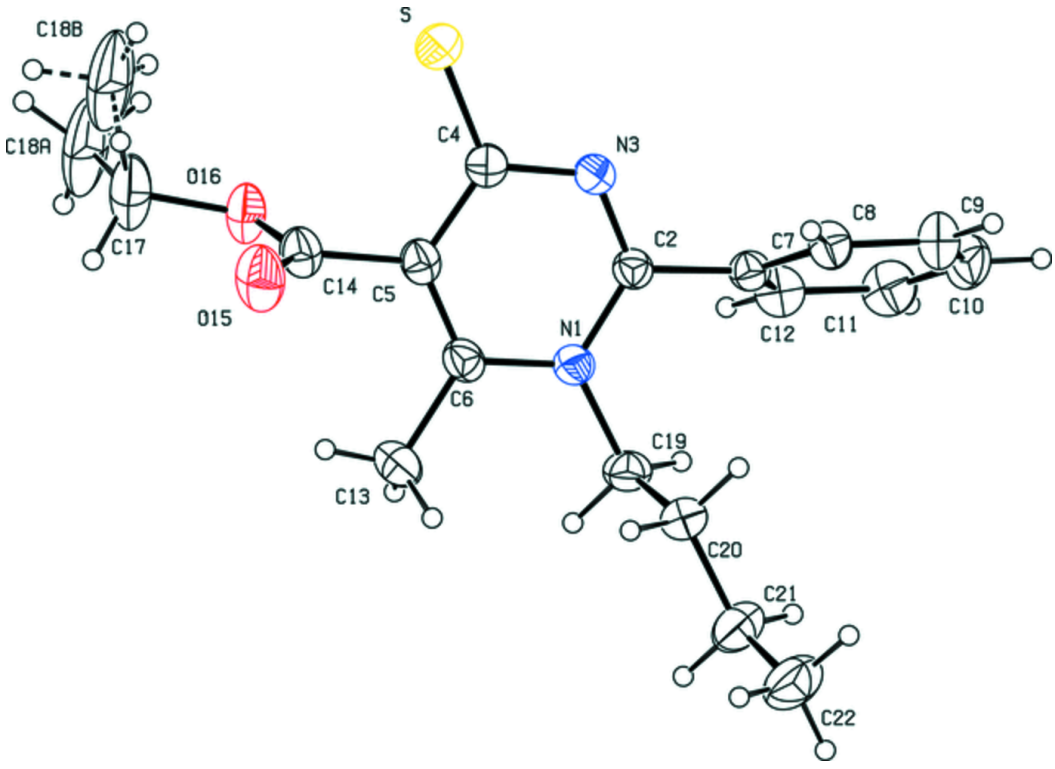
C18B
C18A
C17
O16
O15
C14
C5
S
C4
N3
C2
C7
C8
C9
C10
C11
C12
N1
C6
C13
C19
C20
C21
C22

Fig. 2