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4-Benzyl-5-ethyl-2-(2-furylcarbonylmethylsulfanyl)pyrimidin-6(1*H*)-one

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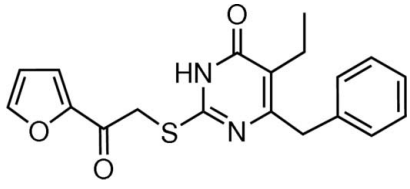
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.051; wR factor = 0.116; data-to-parameter ratio = 18.2.

The title compound, $C_{19}H_{18}N_2O_3S$, shows favourable activity against HIV-1. The phenyl ring is twisted with respect to the pyrimidine ring by 61.56 (9)°. Intermolecular N—H···O and C—H···O hydrogen bonding links the molecules into a supramolecular chain structure and stabilizes the crystal structure of the compound.

Related literature

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



Experimental

Crystal data

$C_{19}H_{18}N_2O_3S$
M_r = 354.41
Monoclinic, $P2_1/c$
a = 12.062 (2) Å
b = 9.3943 (16) Å
c = 15.988 (3) Å
β = 105.065 (2)°
V = 1749.4 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 293 (2) K
0.37 × 0.25 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
11092 measured reflections
4116 independent reflections
2032 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.116
S = 0.99
4116 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O3^{i}	0.86	1.91	2.770 (2)	179
C6—H6B···O2^{ii}	0.97	2.51	3.436 (3)	160

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

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: XU2272).

References

Bruker (1998). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS, Inc., Madison, Wisconsin, USA.
He, Y. P., Chen, F. E., Sun, G. F., Wang, Y. P., De Clercq, E., Balzarini, J. & Pannecouque, C. (2004). *Bioorg. Med. Chem. Lett.* **14**, 3173–3176.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

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4-Benzyl-5-ethyl-2-(2-furylcarbonylmethylsulfanyl)pyrimidin-6(1*H*)-one

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

Comment

As part of our ongoing investigation on the S-DABOs analogues (He *et al.*, 2004), the title compound was synthesized as novel inhibitors and shows favorable activity of anti-HIV-1. Its molecular structure contains a pyrimidine, a furan and a benzene rings (Figure 1). The dihedral angles between the pyrimidine ring and the benzene ring is 61.56 (9)°. The C14—C13—C8 bond angle between the two rings is 117.1 (2)°.

Intermolecular N—H···O and C—H···O hydrogen bonding links the molecules into a chain supra-molecular structure and stabilizes the crystal structure of the compound.

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 wit 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*).

Figures

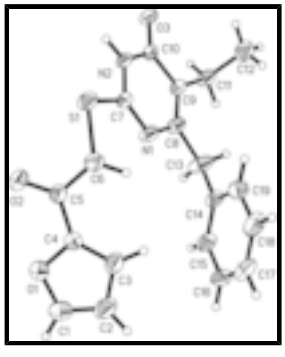

Fig. 1. The molecular structure of the title compound, showing the atom labelling scheme and 30% probability displacement ellipsoids.

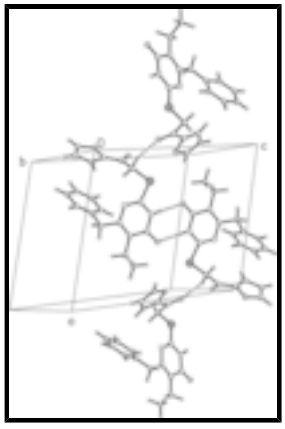

Fig. 2. The crystal packing of title compound showing the intermolecular hydrogen bonding (dotted lines) [symmetry codes: (i) −*x*,-1/2 + *y*,1/2 − *z*; (ii) 1 − *x*,-*y*,1 − *z*].

4-Benzyl-5-ethyl-2-(2-furylcarbonylmethylsulfanyl)pyrimidin-6(1*H*)-one

Crystal data

$C_{19}H_{18}N_2O_3S$	F_{000} = 744
M_r = 354.41	D_x = 1.346 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4116 reflections
a = 12.062 (2) Å	θ = 1.7–28.3º
b = 9.3943 (16) Å	μ = 0.21 mm^{-1}
c = 15.988 (3) Å	*T* = 293 (2) K
β = 105.065 (2)º	Block, colourless
V = 1749.4 (5) Å^3	0.37 × 0.25 × 0.11 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2032 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.054
Monochromator: graphite	θ_{max} = 28.3º
T = 293(2) K	θ_{min} = 1.8º
φ and ω scans	*h* = −16→16
Absorption correction: none	*k* = −12→12
11092 measured reflections	*l* = −20→9
4116 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.051	H-atom parameters constrained

$wR(F^2) = 0.116$	$w = 1/[\sigma^2(F_o^2) + (0.039P)^2]$ where $P = (F_o^2 + 2F_c^2)$
$S = 0.99$	$(\Delta/\sigma)_{max} < 0.001$
4116 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
226 parameters	$\Delta\rho_{min} = -0.21$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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	0.21735 (5)	−0.03809 (8)	0.32866 (4)	0.0558 (2)
O1	−0.03737 (15)	0.3007 (2)	0.10972 (12)	0.0681 (5)
O2	0.03442 (17)	0.1848 (2)	0.26973 (12)	0.0829 (7)
O3	0.61953 (13)	0.05256 (17)	0.45976 (10)	0.0514 (4)
N1	0.36113 (16)	0.0657 (2)	0.23957 (12)	0.0504 (5)
N2	0.43313 (16)	0.02249 (18)	0.38744 (12)	0.0421 (5)
H2A	0.4173	−0.0022	0.4348	0.051*
C1	−0.0516 (3)	0.3368 (3)	0.0258 (2)	0.0769 (9)
H1B	−0.0991	0.4100	−0.0018	0.092*
C2	0.0103 (3)	0.2551 (3)	−0.01204 (19)	0.0767 (9)
H2B	0.0159	0.2617	−0.0688	0.092*
C3	0.0663 (2)	0.1558 (3)	0.05134 (17)	0.0615 (8)
H3A	0.1151	0.0829	0.0439	0.074*
C4	0.0360 (2)	0.1864 (3)	0.12422 (16)	0.0491 (6)
C5	0.0637 (2)	0.1276 (3)	0.21057 (16)	0.0508 (7)
C6	0.1246 (2)	−0.0145 (3)	0.22227 (15)	0.0506 (7)
H6A	0.1695	−0.0227	0.1802	0.061*
H6B	0.0678	−0.0900	0.2108	0.061*
C7	0.34761 (19)	0.0250 (2)	0.31377 (15)	0.0418 (6)
C8	0.4720 (2)	0.1010 (3)	0.23741 (16)	0.0492 (6)
C9	0.56412 (19)	0.0970 (2)	0.30779 (15)	0.0426 (6)
C10	0.5446 (2)	0.0578 (2)	0.38995 (15)	0.0406 (6)
C11	0.68681 (19)	0.1267 (3)	0.30770 (16)	0.0582 (7)
H11A	0.7218	0.1863	0.3570	0.070*
H11B	0.6878	0.1791	0.2556	0.070*
C12	0.7578 (2)	−0.0081 (3)	0.31167 (19)	0.0806 (9)
H12A	0.8350	0.0168	0.3116	0.121*
H12B	0.7248	−0.0666	0.2623	0.121*
H12C	0.7586	−0.0595	0.3637	0.121*

C13	0.4817 (2)	0.1521 (3)	0.14954 (16)	0.0767 (9)
H13A	0.4731	0.2548	0.1477	0.092*
H13B	0.5587	0.1311	0.1451	0.092*
C14	0.3976 (2)	0.0910 (3)	0.07077 (16)	0.0498 (6)
C15	0.3393 (2)	0.1813 (3)	0.00613 (17)	0.0589 (7)
H15A	0.3492	0.2792	0.0128	0.071*
C16	0.2657 (2)	0.1267 (4)	−0.06902 (18)	0.0673 (8)
H16A	0.2272	0.1879	−0.1127	0.081*
C17	0.2502 (3)	−0.0166 (4)	−0.07834 (18)	0.0680 (8)
H17A	0.2005	−0.0533	−0.1282	0.082*
C18	0.3077 (3)	−0.1066 (3)	−0.0144 (2)	0.0749 (9)
H18A	0.2975	−0.2044	−0.0210	0.090*
C19	0.3802 (2)	−0.0527 (3)	0.05903 (19)	0.0654 (8)
H19A	0.4186	−0.1149	0.1021	0.078*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0474 (4)	0.0801 (5)	0.0425 (4)	−0.0032 (4)	0.0163 (3)	0.0115 (4)
O1	0.0748 (12)	0.0766 (13)	0.0550 (13)	0.0235 (11)	0.0208 (10)	0.0094 (11)
O2	0.1038 (15)	0.1021 (16)	0.0484 (12)	0.0378 (13)	0.0300 (12)	−0.0006 (11)
O3	0.0504 (10)	0.0706 (12)	0.0321 (10)	−0.0045 (9)	0.0088 (8)	0.0034 (9)
N1	0.0491 (12)	0.0685 (15)	0.0342 (12)	−0.0081 (10)	0.0117 (10)	0.0093 (10)
N2	0.0493 (12)	0.0508 (12)	0.0291 (11)	−0.0005 (10)	0.0153 (10)	0.0043 (9)
C1	0.086 (2)	0.081 (2)	0.061 (2)	0.0149 (18)	0.0143 (19)	0.0207 (18)
C2	0.100 (2)	0.085 (2)	0.0506 (19)	0.0040 (19)	0.0280 (19)	0.0078 (17)
C3	0.0742 (18)	0.0634 (19)	0.0526 (18)	0.0057 (15)	0.0268 (16)	0.0009 (15)
C4	0.0450 (14)	0.0560 (17)	0.0463 (17)	0.0050 (12)	0.0120 (13)	0.0006 (13)
C5	0.0437 (14)	0.0673 (18)	0.0424 (16)	0.0027 (13)	0.0131 (13)	−0.0042 (14)
C6	0.0459 (14)	0.0622 (17)	0.0412 (15)	−0.0021 (12)	0.0069 (12)	−0.0007 (13)
C7	0.0454 (14)	0.0487 (15)	0.0337 (14)	0.0024 (11)	0.0144 (12)	0.0018 (12)
C8	0.0568 (16)	0.0560 (16)	0.0370 (15)	−0.0091 (13)	0.0163 (13)	0.0067 (12)
C9	0.0487 (14)	0.0475 (15)	0.0336 (14)	−0.0038 (12)	0.0146 (12)	0.0017 (11)
C10	0.0482 (14)	0.0407 (14)	0.0345 (14)	−0.0003 (11)	0.0137 (12)	−0.0007 (11)
C11	0.0505 (15)	0.085 (2)	0.0406 (16)	−0.0124 (15)	0.0144 (13)	0.0047 (14)
C12	0.0637 (19)	0.120 (3)	0.063 (2)	0.0104 (18)	0.0264 (17)	−0.0004 (19)
C13	0.0767 (19)	0.113 (3)	0.0392 (17)	−0.0310 (18)	0.0126 (15)	0.0206 (17)
C14	0.0544 (15)	0.0644 (19)	0.0363 (15)	−0.0039 (13)	0.0220 (13)	0.0119 (14)
C15	0.0814 (19)	0.0544 (17)	0.0454 (17)	−0.0039 (15)	0.0245 (15)	0.0066 (14)
C16	0.075 (2)	0.085 (2)	0.0412 (18)	0.0098 (17)	0.0143 (16)	0.0203 (17)
C17	0.078 (2)	0.089 (2)	0.0405 (18)	−0.0181 (18)	0.0218 (16)	−0.0121 (17)
C18	0.112 (3)	0.061 (2)	0.060 (2)	−0.0046 (19)	0.039 (2)	−0.0063 (18)
C19	0.084 (2)	0.063 (2)	0.056 (2)	0.0123 (16)	0.0294 (17)	0.0170 (16)

Geometric parameters (Å, °)

S1—C7	1.752 (2)	C9—C10	1.442 (3)
S1—C6	1.790 (2)	C9—C11	1.506 (3)
O1—C1	1.350 (3)	C11—C12	1.521 (4)

O1—C4	1.372 (3)	C11—H11A	0.9700
O2—C5	1.217 (3)	C11—H11B	0.9700
O3—C10	1.241 (2)	C12—H12A	0.9600
N1—C7	1.297 (3)	C12—H12B	0.9600
N1—C8	1.387 (3)	C12—H12C	0.9600
N2—C7	1.349 (3)	C13—C14	1.510 (3)
N2—C10	1.375 (3)	C13—H13A	0.9700
N2—H2A	0.8600	C13—H13B	0.9700
C1—C2	1.323 (4)	C14—C19	1.372 (3)
C1—H1B	0.9300	C14—C15	1.380 (3)
C2—C3	1.413 (3)	C15—C16	1.393 (3)
C2—H2B	0.9300	C15—H15A	0.9300
C3—C4	1.340 (3)	C16—C17	1.362 (4)
C3—H3A	0.9300	C16—H16A	0.9300
C4—C5	1.443 (3)	C17—C18	1.368 (4)
C5—C6	1.511 (3)	C17—H17A	0.9300
C6—H6A	0.9700	C18—C19	1.366 (4)
C6—H6B	0.9700	C18—H18A	0.9300
C8—C9	1.361 (3)	C19—H19A	0.9300
C8—C13	1.518 (3)		
C7—S1—C6	100.94 (12)	N2—C10—C9	115.2 (2)
C1—O1—C4	105.9 (2)	C9—C11—C12	112.9 (2)
C7—N1—C8	116.4 (2)	C9—C11—H11A	109.0
C7—N2—C10	122.76 (19)	C12—C11—H11A	109.0
C7—N2—H2A	118.6	C9—C11—H11B	109.0
C10—N2—H2A	118.6	C12—C11—H11B	109.0
C2—C1—O1	111.6 (3)	H11A—C11—H11B	107.8
C2—C1—H1B	124.2	C11—C12—H12A	109.5
O1—C1—H1B	124.2	C11—C12—H12B	109.5
C1—C2—C3	106.0 (3)	H12A—C12—H12B	109.5
C1—C2—H2B	127.0	C11—C12—H12C	109.5
C3—C2—H2B	127.0	H12A—C12—H12C	109.5
C4—C3—C2	107.1 (2)	H12B—C12—H12C	109.5
C4—C3—H3A	126.5	C14—C13—C8	117.1 (2)
C2—C3—H3A	126.5	C14—C13—H13A	108.0
C3—C4—O1	109.3 (2)	C8—C13—H13A	108.0
C3—C4—C5	134.5 (2)	C14—C13—H13B	108.0
O1—C4—C5	116.1 (2)	C8—C13—H13B	108.0
O2—C5—C4	122.1 (2)	H13A—C13—H13B	107.3
O2—C5—C6	121.6 (2)	C19—C14—C15	118.2 (2)
C4—C5—C6	116.2 (2)	C19—C14—C13	122.3 (3)
C5—C6—S1	112.99 (17)	C15—C14—C13	119.5 (3)
C5—C6—H6A	109.0	C14—C15—C16	120.4 (3)
S1—C6—H6A	109.0	C14—C15—H15A	119.8
C5—C6—H6B	109.0	C16—C15—H15A	119.8
S1—C6—H6B	109.0	C17—C16—C15	119.8 (3)
H6A—C6—H6B	107.8	C17—C16—H16A	120.1
N1—C7—N2	123.7 (2)	C15—C16—H16A	120.1
N1—C7—S1	123.68 (18)	C16—C17—C18	120.0 (3)

N2—C7—S1	112.62 (16)	C16—C17—H17A	120.0
C9—C8—N1	123.9 (2)	C18—C17—H17A	120.0
C9—C8—C13	122.1 (2)	C19—C18—C17	120.0 (3)
N1—C8—C13	113.9 (2)	C19—C18—H18A	120.0
C8—C9—C10	117.9 (2)	C17—C18—H18A	120.0
C8—C9—C11	125.8 (2)	C18—C19—C14	121.5 (3)
C10—C9—C11	116.2 (2)	C18—C19—H19A	119.2
O3—C10—N2	119.7 (2)	C14—C19—H19A	119.2
O3—C10—C9	125.2 (2)		
C4—O1—C1—C2	−1.7 (3)	C13—C8—C9—C10	175.1 (2)
O1—C1—C2—C3	1.9 (4)	N1—C8—C9—C11	176.6 (2)
C1—C2—C3—C4	−1.3 (3)	C13—C8—C9—C11	−6.5 (4)
C2—C3—C4—O1	0.3 (3)	C7—N2—C10—O3	−179.6 (2)
C2—C3—C4—C5	−179.3 (3)	C7—N2—C10—C9	−0.4 (3)
C1—O1—C4—C3	0.8 (3)	C8—C9—C10—O3	−178.4 (2)
C1—O1—C4—C5	−179.5 (2)	C11—C9—C10—O3	3.0 (4)
C3—C4—C5—O2	171.6 (3)	C8—C9—C10—N2	2.5 (3)
O1—C4—C5—O2	−7.9 (4)	C11—C9—C10—N2	−176.1 (2)
C3—C4—C5—C6	−12.2 (4)	C8—C9—C11—C12	−102.4 (3)
O1—C4—C5—C6	168.3 (2)	C10—C9—C11—C12	76.1 (3)
O2—C5—C6—S1	−33.7 (3)	C9—C8—C13—C14	151.7 (3)
C4—C5—C6—S1	150.10 (19)	N1—C8—C13—C14	−31.1 (4)
C7—S1—C6—C5	−92.19 (19)	C8—C13—C14—C19	−51.0 (4)
C8—N1—C7—N2	3.4 (4)	C8—C13—C14—C15	131.8 (3)
C8—N1—C7—S1	−174.52 (17)	C19—C14—C15—C16	−0.5 (4)
C10—N2—C7—N1	−2.7 (3)	C13—C14—C15—C16	176.8 (2)
C10—N2—C7—S1	175.38 (16)	C14—C15—C16—C17	0.7 (4)
C6—S1—C7—N1	−3.9 (2)	C15—C16—C17—C18	−0.6 (4)
C6—S1—C7—N2	178.05 (16)	C16—C17—C18—C19	0.4 (4)
C7—N1—C8—C9	−1.0 (4)	C17—C18—C19—C14	−0.2 (4)
C7—N1—C8—C13	−178.2 (2)	C15—C14—C19—C18	0.3 (4)
N1—C8—C9—C10	−1.9 (4)	C13—C14—C19—C18	−176.9 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O3^{i}	0.86	1.91	2.770 (2)	179
C6—H6B···O2^{ii}	0.97	2.51	3.436 (3)	160

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

Fig. 1

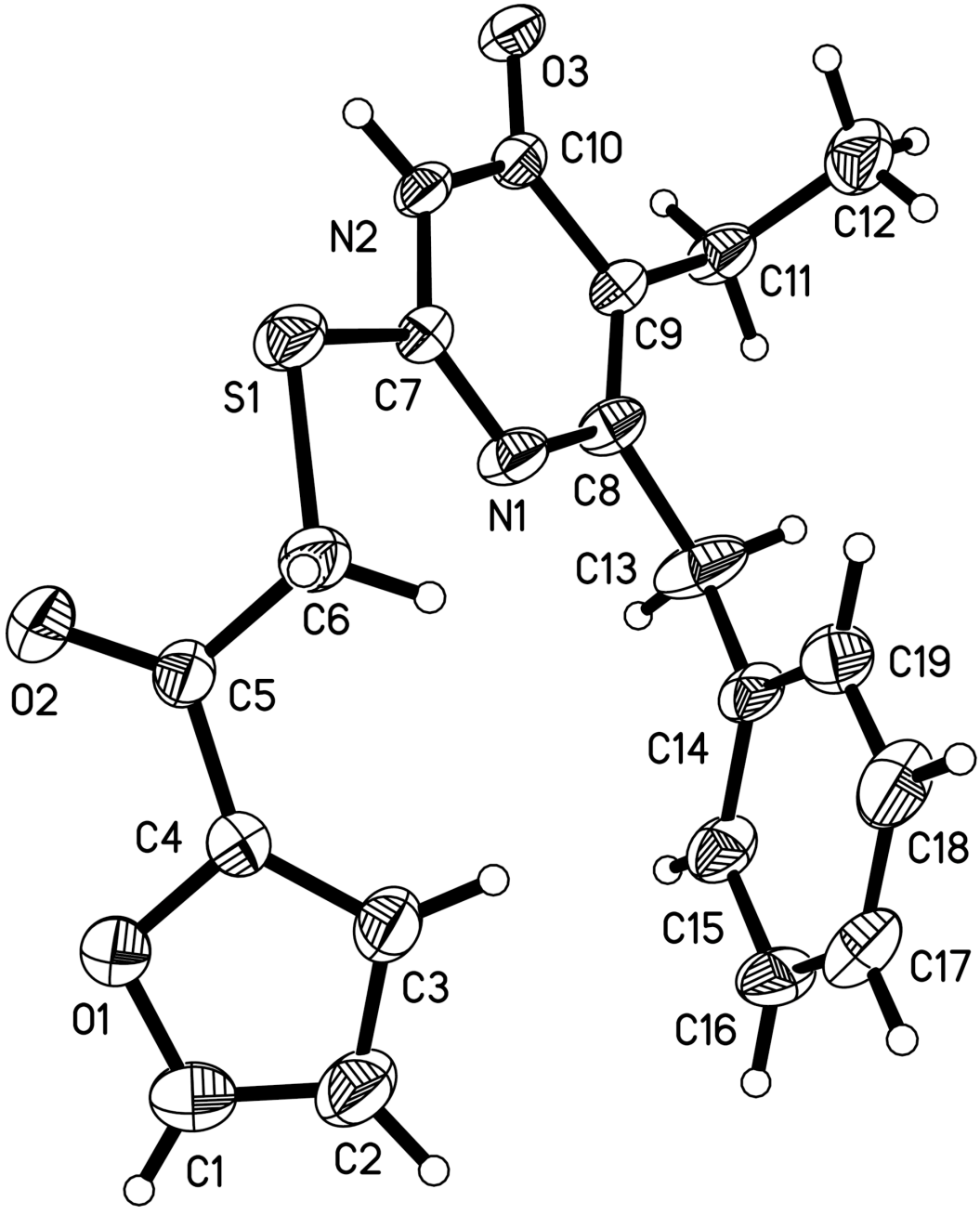
O3
C10
C12
N2
C11
C9
S1
C7
C8
N1
C13
C6
O2
C5
C19
C14
C4
C18
C15
C3
C17
O1
C16
C1
C2

Fig. 2