Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-(2-Furyl)-1-(4-methoxybenzyl)-1*H*-pyrazolo[3,4-*d*]pyrimidine

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Received 27 April 2007; accepted 3 May 2007

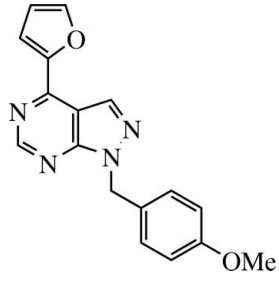
Key indicators: single-crystal X-ray study; T = 112 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.135; data-to-parameter ratio = 15.2.

The title compound, $C_{17}H_{14}N_4O_2$, is a close analog of potent antimycobacterial purines. Molecules are linked by C—H···N hydrogen bonds, forming infinite chains along [010]. The secondary structure is further stabilized by weak intermolecular contacts of types C—H···N and C—H···O.

Related literature

Most bond lengths and angles are in good agreement with those found for 6-furyl- and 6-thienyl-9-benzylpurines (Braendvang & Gundersen, 2007*a*; Mazumdar *et al.*, 2001), except that the furyl ring in the title compound is rotated by approximately 180°. This orientation of the furyl ring is stabilized by C—H···O hydrogen bonding.

For related literature, see: Bakkestuen *et al.* (2000, 2005); Brændvang & Gundersen (2005, 2007*b*); Gundersen *et al.* (2002).



Experimental

Crystal data

$C_{17}H_{14}N_4O_2$
M_r = 306.32
Triclinic, $P\overline{1}$
a = 8.2163 (15) Å
b = 8.4765 (15) Å
c = 12.437 (2) Å
α = 72.485 (3)°
β = 74.209 (3)°
γ = 61.065 (3)°
V = 714.6 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 112 (2) K
0.20 × 0.20 × 0.15 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.661, T_{max} = 0.986
5825 measured reflections
3187 independent reflections
2422 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.135
S = 1.03
3187 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C21—H21···N2^{i}	0.95	2.41	3.338 (2)	164
C16—H16A···N7^{ii}	0.98	2.60	3.572 (2)	174
C3—H3···O18	0.95	2.60	3.029 (2)	108
C6—H6···O15^{iii}	0.95	2.51	3.344 (2)	147

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

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: *ORTEP-3 for Windows* (Farrugia, 1997) and *POV-RAY for Windows* (Persistence of Vision Pty. Ltd, 2004); software used to prepare material for publication: *SHELXL97* and *WinGX* (Farrugia, 1999).

The authors thank Dr Osamu Sekiguchi, Department of Chemistry, University of Oslo, for the single-crystal data collection and initial refinement.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2248).

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 doi:10.1107/S1600536807021952

supplementary materials

Acta Cryst. (2007). E**63**, o2849 [**doi:10.1107/S1600536807021952**]

4-(2-Furyl)-1-(4-methoxybenzyl)-1*H*-pyrazolo[3,4-*d*]pyrimidine

M. Brændvang and L.-L. Gundersen

Comment

We have discovered that certain 6-aryl-9-benzylpurines are potent antimycobacterials *in vitro* and may have a potential as antitubercular drugs (Bakkestuen *et al.*, 2000; Gundersen *et al.*, 2002; Bakkestuen *et al.*, 2005; Braendvang & Gundersen, 2005). Compound **I** was synthesised as a non-purine analog of the previously reported antimycobacterial purines (Braendvang & Gundersen, 2007 b).

The molecular geometries are illustrated in Fig. 1 and the bond lengths and angles are listed in Table 1. The angle between the mean plane of the pyrazolo-pyrimidine ring system and the furyl ring are 0.66 (8)°. This coplanarity has also been reported for 6-arylpurines, except that the furyl ring in compound **I** is rotated approximately 180° compared to previously reported purine structure (Braendvang & Gundersen, 2007a). The orientation of the furyl group is stabilized by intramolecular C3–H3···O18 hydrogen bonding (Table 2). The benzene ring plane is inclined at an angle of 72.83 (7)° to the pyrazolo-pyrimidine ring system, and is very similar as in case of purine ring system previously reported (Braendvang & Gundersen, 2007a).

Fig. 2. shows the molecules in the unit cell. The molecular packing is similar to previous reported purine analog (Braendvang & Gundersen, 2007a), except that the infinite chain along [010] is linked together by hydrogen bonding C21–H21···N2^{i} [Table 2 and Fig. 2; symmetry code: (i) x, y-1, z] while in the previous reported structure the hydrogen bonding is between the oxygen in the furyl ring and the H8 in the purine ring.

Experimental

The title compound was synthesized as described by Brændvang & Gundersen (2007 b). Crystals suitable for X-ray diffraction studies were obtained by slow evaporation at room temperature from a mixture of acetone and hexane (1:2).

Refinement

H atoms were positioned geometrically and allowed to ride and rotate (for the CH_3 group) on their carrier atoms, with C—H bond lengths of 0.95 (aromatic C—H), 0.99 (CH_2) or 0.98 Å (CH_3) and with $U_{iso}(H) = 1.2U_{eq}(C)$ for methylene and aromatic C—H or $1.5U_{eq}(C)$ for CH_3.

Figures

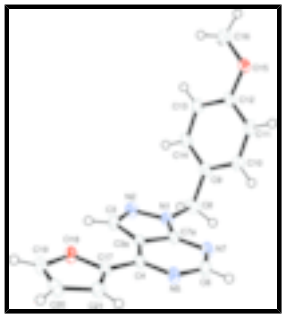

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

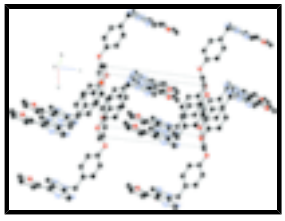

Fig. 2. The packing of (I), viewed down the *b* axis, showing the infinite chains of (I) along *b* axis. H atoms have been omitted for clarity.

4-(2-Furyl)-1-(4-methoxybenzyl)-1*H*-pyrazolo[3,4,d]pyrimidine

Crystal data

$C_{17}H_{14}N_4O_2$	$Z = 2$
$M_r = 306.32$	$F_{000} = 320$
Triclinic, $P\bar{1}$	$D_x = 1.424$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.2163$ (15) Å	Cell parameters from 2969 reflections
$b = 8.4765$ (15) Å	$\theta = 2.8$–28.3º
$c = 12.437$ (2) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 72.485$ (3)º	$T = 112$ (2) K
$\beta = 74.209$ (3)º	Block, yellow
$\gamma = 61.065$ (3)º	0.20 × 0.20 × 0.15 mm
$V = 714.6$ (2) Å^3	

Data collection

Siemens SMART CCD diffractometer	$R_{int} = 0.025$
ω scans	$\theta_{max} = 28.8$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{min} = 1.7$º
$T_{min} = 0.661$, $T_{max} = 0.986$	$h = -10 \rightarrow 9$
5825 measured reflections	$k = -10 \rightarrow 11$
3187 independent reflections	$l = -15 \rightarrow 16$
2422 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.135$

$S = 1.03$

3187 reflections

210 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0927P)^2]$

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

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.29$ e Å^{-3}

$\Delta\rho_{min} = -0.30$ e Å^{-3}

Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.009 (5)

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}
C16	0.0212 (2)	1.2299 (2)	1.00299 (13)	0.0310 (4)
H16B	−0.0885	1.2588	1.0631	0.046*
H16A	−0.0199	1.2561	0.93	0.046*
H16C	0.0847	1.3052	0.9974	0.046*
C12	0.3085 (2)	0.9750 (2)	0.95405 (12)	0.0219 (3)
C13	0.3569 (2)	1.0823 (2)	0.85326 (12)	0.0246 (3)
H13	0.2734	1.2083	0.8316	0.03*
C14	0.5284 (2)	1.0031 (2)	0.78483 (12)	0.0243 (3)
H14	0.5622	1.0772	0.7172	0.029*
C9	0.6511 (2)	0.8187 (2)	0.81324 (12)	0.0227 (3)
C10	0.5980 (2)	0.7109 (2)	0.91305 (12)	0.0249 (3)
H10	0.6788	0.5835	0.933	0.03*
C11	0.4287 (2)	0.7889 (2)	0.98257 (12)	0.0254 (3)
H11	0.3944	0.7149	1.0501	0.03*
C8	0.8340 (2)	0.7353 (2)	0.73554 (13)	0.0277 (4)
H8B	0.8838	0.8279	0.7005	0.033*
H8A	0.9272	0.6296	0.7814	0.033*
C3	0.7299 (2)	0.7047 (2)	0.48624 (12)	0.0238 (3)
H3	0.6905	0.7563	0.4133	0.029*
C3A	0.7731 (2)	0.5197 (2)	0.54462 (11)	0.0199 (3)
C4	0.7772 (2)	0.3590 (2)	0.53073 (11)	0.0201 (3)
C6	0.8695 (2)	0.2165 (2)	0.70764 (12)	0.0277 (4)
H6	0.9036	0.1068	0.7644	0.033*

C7A	0.8228 (2)	0.5069 (2)	0.64762 (12)	0.0212 (3)
C17	0.7315 (2)	0.3450 (2)	0.43035 (11)	0.0209 (3)
C19	0.6430 (2)	0.4520 (2)	0.26199 (13)	0.0283 (4)
H19	0.6031	0.5326	0.1925	0.034*
C20	0.6719 (2)	0.2745 (2)	0.29123 (12)	0.0279 (4)
H20	0.6569	0.2094	0.2473	0.033*
C21	0.7291 (2)	0.2044 (2)	0.40082 (12)	0.0249 (3)
H21	0.7595	0.0833	0.4447	0.03*
N1	0.81128 (18)	0.67308 (17)	0.64542 (10)	0.0239 (3)
N2	0.75177 (19)	0.79507 (17)	0.54690 (10)	0.0260 (3)
N5	0.82546 (19)	0.20712 (17)	0.61400 (10)	0.0251 (3)
N7	0.87220 (19)	0.35803 (18)	0.73238 (10)	0.0256 (3)
O15	0.14786 (15)	1.04026 (15)	1.02991 (8)	0.0279 (3)
O18	0.67872 (15)	0.50055 (14)	0.34530 (8)	0.0254 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C16	0.0294 (9)	0.0345 (9)	0.0258 (8)	−0.0120 (8)	−0.0011 (7)	−0.0081 (7)
C12	0.0244 (8)	0.0289 (8)	0.0170 (6)	−0.0158 (7)	−0.0021 (6)	−0.0044 (6)
C13	0.0308 (9)	0.0220 (8)	0.0221 (7)	−0.0144 (7)	−0.0035 (6)	−0.0012 (6)
C14	0.0331 (9)	0.0273 (8)	0.0190 (7)	−0.0208 (7)	−0.0018 (6)	−0.0018 (6)
C9	0.0267 (8)	0.0288 (8)	0.0210 (7)	−0.0172 (7)	−0.0035 (6)	−0.0075 (6)
C10	0.0295 (8)	0.0226 (8)	0.0240 (7)	−0.0118 (7)	−0.0087 (6)	−0.0015 (6)
C11	0.0316 (9)	0.0293 (8)	0.0175 (6)	−0.0183 (7)	−0.0061 (6)	0.0030 (6)
C8	0.0272 (8)	0.0357 (9)	0.0288 (8)	−0.0184 (7)	−0.0011 (6)	−0.0128 (7)
C3	0.0287 (8)	0.0240 (8)	0.0193 (7)	−0.0152 (7)	−0.0024 (6)	0.0000 (6)
C3A	0.0218 (7)	0.0218 (7)	0.0161 (6)	−0.0121 (6)	−0.0004 (5)	−0.0017 (5)
C4	0.0224 (7)	0.0216 (7)	0.0168 (6)	−0.0130 (6)	0.0002 (5)	−0.0012 (5)
C6	0.0370 (9)	0.0261 (8)	0.0181 (7)	−0.0160 (7)	−0.0045 (6)	0.0023 (6)
C7A	0.0225 (8)	0.0243 (8)	0.0183 (7)	−0.0133 (6)	0.0010 (6)	−0.0044 (6)
C17	0.0225 (8)	0.0230 (8)	0.0172 (6)	−0.0135 (6)	−0.0009 (6)	0.0000 (6)
C19	0.0331 (9)	0.0377 (9)	0.0190 (7)	−0.0202 (8)	−0.0055 (6)	−0.0028 (6)
C20	0.0329 (9)	0.0377 (9)	0.0223 (7)	−0.0229 (8)	−0.0005 (6)	−0.0088 (7)
C21	0.0300 (8)	0.0260 (8)	0.0220 (7)	−0.0169 (7)	−0.0008 (6)	−0.0037 (6)
N1	0.0294 (7)	0.0250 (7)	0.0210 (6)	−0.0157 (6)	−0.0024 (5)	−0.0044 (5)
N2	0.0321 (7)	0.0233 (7)	0.0239 (6)	−0.0159 (6)	−0.0029 (5)	−0.0012 (5)
N5	0.0339 (7)	0.0239 (7)	0.0184 (6)	−0.0166 (6)	−0.0032 (5)	0.0009 (5)
N7	0.0327 (7)	0.0269 (7)	0.0176 (6)	−0.0151 (6)	−0.0046 (5)	−0.0007 (5)
O15	0.0262 (6)	0.0327 (6)	0.0193 (5)	−0.0124 (5)	−0.0004 (4)	−0.0016 (4)
O18	0.0357 (6)	0.0242 (6)	0.0185 (5)	−0.0168 (5)	−0.0071 (4)	0.0019 (4)

Geometric parameters (Å, °)

C16—O15	1.423 (2)	C3—N2	1.3199 (19)
C16—H16B	0.98	C3—C3A	1.425 (2)
C16—H16A	0.98	C3—H3	0.95
C16—H16C	0.98	C3A—C7A	1.4063 (19)
C12—O15	1.3669 (18)	C3A—C4	1.407 (2)

C12—C11	1.392 (2)	C4—N5	1.3470 (18)
C12—C13	1.396 (2)	C6—N7	1.336 (2)
C13—C14	1.392 (2)	C6—N5	1.344 (2)
C13—H13	0.95	C6—H6	0.95
C14—C9	1.386 (2)	C7A—N7	1.3437 (18)
C14—H14	0.95	C7A—N1	1.3574 (18)
C9—C10	1.405 (2)	C17—C21	1.358 (2)
N1—C8	1.4610 (18)	C17—O18	1.3793 (16)
C4—C17	1.4494 (19)	C19—C20	1.351 (2)
C8—C9	1.512 (2)	C19—O18	1.3667 (18)
C10—C11	1.385 (2)	C19—H19	0.95
C10—H10	0.95	C20—C21	1.422 (2)
C11—H11	0.95	C20—H20	0.95
C8—H8B	0.99	C21—H21	0.95
C8—H8A	0.99	N1—N2	1.3726 (17)
O15—C16—H16B	109.5	C7A—C3A—C4	115.70 (13)
O15—C16—H16A	109.5	C7A—C3A—C3	104.23 (12)
H16B—C16—H16A	109.5	C4—C3A—C3	140.06 (13)
O15—C16—H16C	109.5	N5—C4—C3A	119.68 (13)
H16B—C16—H16C	109.5	N5—C4—C17	116.53 (13)
H16A—C16—H16C	109.5	C3A—C4—C17	123.80 (13)
O15—C12—C11	115.94 (13)	N7—C6—N5	129.32 (14)
O15—C12—C13	124.37 (14)	N7—C6—H6	115.3
C11—C12—C13	119.68 (14)	N5—C6—H6	115.3
C14—C13—C12	119.47 (14)	N7—C7A—N1	126.44 (13)
C14—C13—H13	120.3	N7—C7A—C3A	126.35 (13)
C12—C13—H13	120.3	N1—C7A—C3A	107.22 (13)
C9—C14—C13	121.45 (14)	C21—C17—O18	110.44 (12)
C9—C14—H14	119.3	C21—C17—C4	132.49 (14)
C13—C14—H14	119.3	O18—C17—C4	117.07 (12)
C14—C9—C10	118.51 (14)	C20—C19—O18	111.19 (13)
C14—C9—C8	120.25 (14)	C20—C19—H19	124.4
C10—C9—C8	121.19 (14)	O18—C19—H19	124.4
C11—C10—C9	120.49 (15)	C19—C20—C21	106.41 (13)
C11—C10—H10	119.8	C19—C20—H20	126.8
C9—C10—H10	119.8	C21—C20—H20	126.8
C10—C11—C12	120.35 (14)	C17—C21—C20	106.38 (13)
C10—C11—H11	119.8	C17—C21—H21	126.8
C12—C11—H11	119.8	C20—C21—H21	126.8
N1—C8—C9	112.29 (12)	C7A—N1—N2	110.83 (12)
N1—C8—H8B	109.1	C7A—N1—C8	128.64 (13)
C9—C8—H8B	109.1	N2—N1—C8	120.17 (12)
N1—C8—H8A	109.1	C3—N2—N1	106.67 (12)
C9—C8—H8A	109.1	C6—N5—C4	117.58 (13)
H8B—C8—H8A	107.9	C6—N7—C7A	111.38 (12)
N2—C3—C3A	111.02 (13)	C12—O15—C16	117.41 (12)
N2—C3—H3	124.5	C19—O18—C17	105.58 (11)
C3A—C3—H3	124.5		

O15—C12—C13—C14	177.07 (13)	C3A—C4—C17—O18	−1.0 (2)
C11—C12—C13—C14	−2.6 (2)	O18—C19—C20—C21	0.29 (18)
C12—C13—C14—C9	1.4 (2)	O18—C17—C21—C20	0.04 (17)
C13—C14—C9—C10	0.6 (2)	C4—C17—C21—C20	179.89 (15)
C13—C14—C9—C8	178.30 (13)	C19—C20—C21—C17	−0.20 (17)
C14—C9—C10—C11	−1.5 (2)	N7—C7A—N1—N2	−178.42 (13)
C8—C9—C10—C11	−179.15 (13)	C3A—C7A—N1—N2	1.53 (16)
C9—C10—C11—C12	0.3 (2)	N7—C7A—N1—C8	−5.4 (2)
O15—C12—C11—C10	−177.94 (12)	C3A—C7A—N1—C8	174.58 (14)
C13—C12—C11—C10	1.7 (2)	C9—C8—N1—C7A	−88.40 (19)
C14—C9—C8—N1	−85.88 (17)	C9—C8—N1—N2	84.09 (17)
C10—C9—C8—N1	91.74 (17)	C3A—C3—N2—N1	0.61 (17)
N2—C3—C3A—C7A	0.28 (17)	C7A—N1—N2—C3	−1.34 (16)
N2—C3—C3A—C4	179.00 (18)	C8—N1—N2—C3	−175.07 (13)
C7A—C3A—C4—N5	0.4 (2)	N7—C6—N5—C4	0.4 (3)
C3—C3A—C4—N5	−178.22 (17)	C3A—C4—N5—C6	−0.5 (2)
C7A—C3A—C4—C17	−179.69 (13)	C17—C4—N5—C6	179.62 (13)
C3—C3A—C4—C17	1.7 (3)	N5—C6—N7—C7A	−0.2 (2)
C4—C3A—C7A—N7	−0.2 (2)	N1—C7A—N7—C6	−179.97 (14)
C3—C3A—C7A—N7	178.87 (14)	C3A—C7A—N7—C6	0.1 (2)
C4—C3A—C7A—N1	179.84 (12)	C11—C12—O15—C16	−179.58 (13)
C3—C3A—C7A—N1	−1.08 (16)	C13—C12—O15—C16	0.8 (2)
N5—C4—C17—C21	−0.9 (2)	C20—C19—O18—C17	−0.27 (17)
C3A—C4—C17—C21	179.19 (15)	C21—C17—O18—C19	0.13 (16)
N5—C4—C17—O18	178.94 (12)	C4—C17—O18—C19	−179.74 (13)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C21—H21···N2^{i}	0.95	2.41	3.338 (2)	164
C16—H16A···N7^{ii}	0.98	2.60	3.572 (2)	174
C3—H3···O18	0.95	2.60	3.029 (2)	108
C6—H6···O15^{iii}	0.95	2.51	3.344 (2)	147

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

Fig. 1

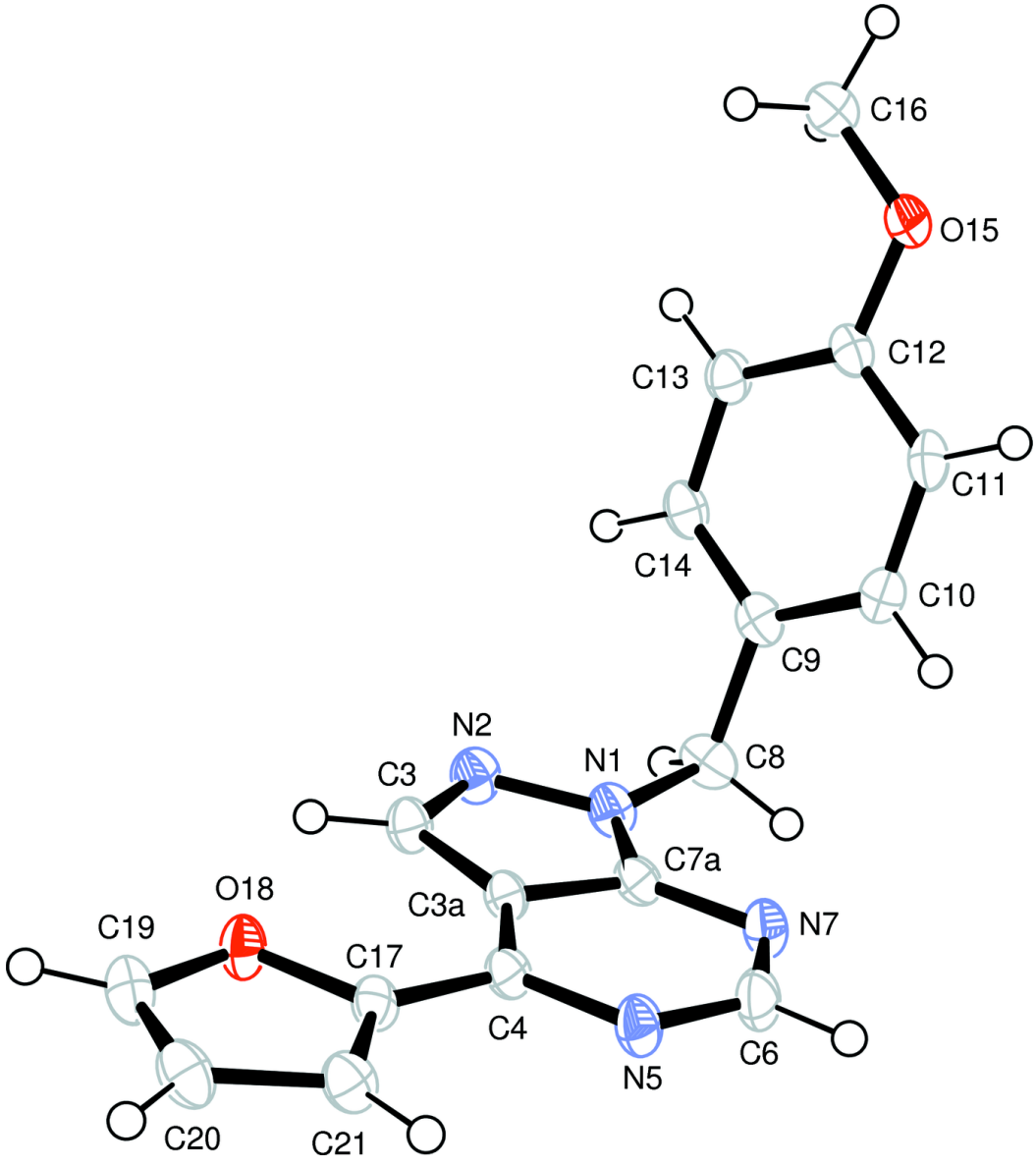
C16
O15
C12
C13
C11
C14
C10
C9
N2
N1
C8
C3
C7a
O18
C3a
N7
C19
C17
C4
C6
N5
C20
C21

Fig. 2