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N-(4,6-Dimethoxypyrimidin-2-yl)-2-(3-methylphenyl)acetamide

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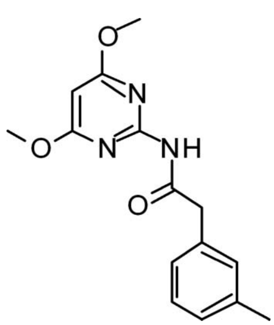
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.132; data-to-parameter ratio = 24.0.

In the title compound, $C_{15}H_{17}N_3O_3$, the dihedral angle between the pyrimidine and benzene rings is 87.0 (7)°. In the crystal, molecules are linked into inversion dimers with $R_2^2(8)$ graph-set motifs by a pair of N—H$\cdots$O hydrogen bonds. Weak C—H$\cdots$O hydrogen bonds and intermolecular π–π interactions [centroid–centroid distance = 3.544 (1) Å] are also observed.

Related literature

For the pyrimidine ring in vitamins, see: Cox (1968). For barbitone, the first barbiturate hypnotic sedative, see: Russell (1945). For the similarity of related *N*-substituted 2-aryl-acetamides to the lateral chain of natural benzylpenicillin, see: Mijin & Marinkovic (2006); Mijin *et al.* (2008). For the coordination abilities of amides, see: Wu *et al.* (2008, 2010). For related structures, see: John *et al.* (2010); Nogueira *et al.* (2010); Praveen *et al.* (2011); Selig *et al.* (2010); Wen *et al.* (2010). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{15}H_{17}N_3O_3$
M_r = 287.32
Triclinic, $P\bar{1}$
a = 7.1536 (6) Å
b = 8.2070 (7) Å
c = 13.8259 (10) Å
α = 74.420 (7)°
β = 86.540 (6)°
γ = 69.186 (8)°
V = 730.30 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 173 K
0.42 × 0.34 × 0.22 mm

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
T_{min} = 0.961, T_{max} = 0.980
8350 measured reflections
4735 independent reflections
3887 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.132
S = 1.02
4735 reflections
197 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D\cdots A$	D—H$\cdots$$A$
N3—H3$N\cdots$O3^{i}	0.875 (15)	1.979 (15)	2.8535 (12)	176.0 (14)
C3—H3$\cdots$O2^{ii}	0.93	2.52	3.4459 (12)	177

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: IS5034).

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supplementary materials

Acta Cryst. (2012). E**68**, o226-o227 [doi:10.1107/S1600536811054493]

N-(4,6-Dimethoxypyrimidin-2-yl)-2-(3-methylphenyl)acetamide

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Comment

The pyrimidine ring is found in vitamins like thiamine, riboflavin and folic acid (Cox, 1968). Barbitone, the first barbiturate hypnotic sedative and anticonvulsant, is a pyrimidine derivative (Russell, 1945). N-Substituted 2-arylacetamides are very interesting compounds because of their structural similarity to the lateral chain of natural benzylpenicillin (Mijin *et al.*, 2006, 2008). Amides are also used as ligands due to their excellent coordination abilities (Wu *et al.*, 2008, 2010).

Crystal structures of some acetamidederivatives, *viz*., 2-[(5,7-dibromoquinolin-8-yl)oxy]-N-(2-methoxyphenyl)acetamide (Wen *et al.*, 2010), N-(4-bromophenyl)-2-(2-thienyl)acetamide (Nogueira *et al.*, 2010), N-[4-(benzylsulfamoyl)phenyl]acetamide (John *et al.*, 2010), 2-(4-fluorophenyl)-N-{4-[6-(4-fluorophenyl)-2,3-dihydroimidazo [2,1-b][1,3]thiazol-5-yl]pyridin-2-yl}acetamide (Selig *et al.*, 2010) and recently from our laboratories, N-(3-chloro-4-fluorophenyl)-2-(naphthalen-1-yl)acetamide (Praveen *et al.*, 2011) have been reported. As part of our ongoing studies of amides, the title compound is synthesized and its crystal structure is reported.

In the crystal structure of the title compound, $C_{15}H_{17}N_3O_3$, the dihedral angle between the pyrimidine and benzene rings is 93.0 (7)° (Fig. 1). Bond lengths are in normal ranges (Allen *et al.*, 1987). Crystal packing is stabilized by N—H···O hydrogen bonds forming an $R^2_2(8)$ graph-set motif (Fig. 2). Weak C—H···O (Table 1) and π—π intermolecular interactions [centroid-centroid distance = 3.544 (1) Å] are also observed.

Experimental

To a stirred solution of (3-methylphenyl)acetic acid (1 g, 6.65 mmol), triethylamine (1.34 g, 13.31 mmol) and 4,6-dimethoxypyrimidin-2-amine (1.02 g, 6.65 mmol) in dichloromethane (10 ml), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide HCl (1.52 g, 7.93 mmol) was added at 273 K. Reaction mixture was stirred at room temperature for 3 h. After the completion of the reaction, the reaction mixture was poured to ice cold water and the layers were separated. Organic layer was washed with 10% aq.$NaHCO_3$ solution (10 ml), brine (10 ml), dried over anhydrous Na_2SO_4, filtered and concentrated under vacuum to obtain the crude product which was triturated with ethanol and filtered to afford 1.62 g of the title compound (I) as a white solid in 84% yield. Single crystals were grown from ethanol by the slow evaporation method (m.p. 381-382 K).

Refinement

Atom H3N was located in a difference Fourier map and refined isotropically. All of the remaining H atoms were placed in their calculated positions and then refined using the riding model with C—H = 0.93 Å (CH), 0.97 Å (CH_2) or 0.96 Å (CH_3). The U_{iso}(H) values were set to 1.2 (CH, CH_2) or 1.5 CH_3) times U_{eq} of the parent atom.

Figures

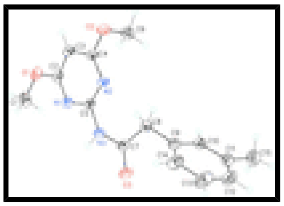

Fig. 1. Molecular structure of the title compound, showing the atom labeling scheme and 50% probability displacement ellipsoids.

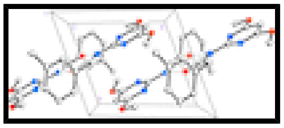

Fig. 2. Packing diagram of the title compound viewed along the *c* axis. Dashed line represent N—H···O hydrogen bonds forming an $R^2_2(8)$ graph-set motif. The remaining H atoms have been removed for clarity.

N-(4,6-Dimethoxypyrimidin-2-yl)-2-(3-methylphenyl)acetamide

Crystal data

$C_{15}H_{17}N_3O_3$	$Z = 2$
$M_r = 287.32$	$F(000) = 304$
Triclinic, $P\bar{1}$	$D_x = 1.306$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.1536$ (6) Å	Cell parameters from 3427 reflections
$b = 8.2070$ (7) Å	$\theta = 3.1–32.3°$
$c = 13.8259$ (10) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 74.420$ (7)°	$T = 173$ K
$\beta = 86.540$ (6)°	Chunk, colorless
$\gamma = 69.186$ (8)°	0.42 × 0.34 × 0.22 mm
$V = 730.30$ (10) Å^3	

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer	4735 independent reflections
Radiation source: Enhance (Mo) X-ray Source	3887 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.020$
Detector resolution: 16.1500 pixels mm^{-1}	$\theta_{max} = 32.3°$, $\theta_{min} = 3.1°$
ω scans	$h = -10\rightarrow10$
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)	$k = -10\rightarrow12$
$T_{min} = 0.961$, $T_{max} = 0.980$	$l = -20\rightarrow20$
8350 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.047$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.132$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.0664P)^2 + 0.156P]$ where $P = (F_o^2 + 2F_c^2)/3$
4735 reflections	$(\Delta/\sigma)_{max} < 0.001$
197 parameters	$\Delta\rho_{max} = 0.37$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.22$ e Å^{-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.

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 $F^2 > \sigma(F^2)$ 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}
O1	0.53082 (13)	0.72818 (11)	−0.19967 (6)	0.03281 (19)
O2	0.68411 (13)	0.78056 (10)	0.11132 (7)	0.03380 (19)
O3	1.08112 (15)	−0.05781 (10)	0.12226 (7)	0.0384 (2)
N1	0.71599 (12)	0.47480 (11)	−0.07942 (6)	0.02315 (17)
N2	0.79478 (12)	0.50033 (10)	0.08008 (6)	0.02230 (17)
N3	0.90035 (13)	0.22301 (11)	0.03696 (7)	0.02455 (18)
H3N	0.902 (2)	0.177 (2)	−0.0136 (11)	0.029 (3)*
C1	0.5650 (2)	0.60945 (19)	−0.26389 (9)	0.0382 (3)
H1A	0.7060	0.5570	−0.2723	0.057*
H1B	0.4987	0.6768	−0.3282	0.057*
H1C	0.5130	0.5152	−0.2340	0.057*
C2	0.61661 (14)	0.65189 (13)	−0.10610 (8)	0.0241 (2)
C3	0.59691 (16)	0.76447 (13)	−0.04444 (8)	0.0276 (2)
H3	0.5249	0.8880	−0.0642	0.033*
C4	0.69324 (15)	0.67809 (13)	0.04902 (8)	0.02425 (19)
C5	0.79884 (13)	0.40869 (12)	0.01346 (7)	0.02076 (18)
C6	0.80040 (19)	0.69559 (16)	0.20397 (9)	0.0340 (2)
H6A	0.7555	0.6020	0.2436	0.051*
H6B	0.7846	0.7839	0.2404	0.051*
H6C	0.9389	0.6440	0.1900	0.051*
C7	0.99644 (15)	0.09987 (13)	0.12367 (8)	0.0244 (2)
C8	0.99476 (16)	0.15771 (13)	0.21836 (8)	0.0254 (2)
H8A	1.0698	0.2384	0.2088	0.030*

H8B	0.8580	0.2239	0.2317	0.030*
C9	1.08408 (16)	−0.00098 (13)	0.30737 (8)	0.0268 (2)
C10	0.96179 (18)	−0.06648 (14)	0.37637 (8)	0.0291 (2)
H10	0.8237	−0.0125	0.3662	0.035*
C11	1.0405 (2)	−0.21160 (16)	0.46093 (9)	0.0365 (3)
C12	1.2469 (2)	−0.28988 (17)	0.47418 (10)	0.0465 (3)
H12	1.3028	−0.3863	0.5299	0.056*
C13	1.3710 (2)	−0.22672 (19)	0.40569 (13)	0.0509 (4)
H13	1.5091	−0.2811	0.4158	0.061*
C14	1.29121 (19)	−0.08320 (17)	0.32224 (11)	0.0395 (3)
H14	1.3754	−0.0418	0.2763	0.047*
C15	0.9033 (3)	−0.2773 (2)	0.53551 (11)	0.0532 (4)
H15A	0.8517	−0.3510	0.5095	0.080*
H15B	0.7944	−0.1755	0.5467	0.080*
H15C	0.9765	−0.3474	0.5978	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0345 (4)	0.0291 (4)	0.0288 (4)	−0.0088 (3)	−0.0081 (3)	0.0008 (3)
O2	0.0394 (4)	0.0197 (3)	0.0398 (5)	−0.0029 (3)	−0.0054 (3)	−0.0126 (3)
O3	0.0558 (5)	0.0174 (3)	0.0345 (4)	−0.0007 (3)	−0.0127 (4)	−0.0084 (3)
N1	0.0225 (4)	0.0204 (4)	0.0253 (4)	−0.0070 (3)	−0.0003 (3)	−0.0044 (3)
N2	0.0225 (4)	0.0166 (3)	0.0269 (4)	−0.0053 (3)	0.0003 (3)	−0.0064 (3)
N3	0.0291 (4)	0.0165 (3)	0.0264 (4)	−0.0042 (3)	−0.0036 (3)	−0.0072 (3)
C1	0.0366 (6)	0.0473 (7)	0.0269 (5)	−0.0117 (5)	−0.0025 (4)	−0.0072 (5)
C2	0.0207 (4)	0.0226 (4)	0.0264 (5)	−0.0082 (3)	−0.0015 (3)	−0.0007 (4)
C3	0.0272 (5)	0.0162 (4)	0.0343 (5)	−0.0042 (3)	−0.0032 (4)	−0.0021 (4)
C4	0.0231 (4)	0.0177 (4)	0.0315 (5)	−0.0058 (3)	0.0008 (4)	−0.0077 (4)
C5	0.0192 (4)	0.0170 (4)	0.0257 (4)	−0.0065 (3)	0.0009 (3)	−0.0049 (3)
C6	0.0396 (6)	0.0300 (5)	0.0348 (6)	−0.0103 (5)	−0.0018 (5)	−0.0148 (4)
C7	0.0264 (5)	0.0181 (4)	0.0277 (5)	−0.0061 (3)	−0.0028 (4)	−0.0061 (3)
C8	0.0285 (5)	0.0194 (4)	0.0254 (5)	−0.0042 (4)	−0.0018 (4)	−0.0066 (3)
C9	0.0311 (5)	0.0195 (4)	0.0272 (5)	−0.0044 (4)	−0.0052 (4)	−0.0067 (4)
C10	0.0358 (5)	0.0253 (5)	0.0268 (5)	−0.0091 (4)	−0.0025 (4)	−0.0092 (4)
C11	0.0591 (8)	0.0274 (5)	0.0258 (5)	−0.0168 (5)	−0.0020 (5)	−0.0084 (4)
C12	0.0640 (9)	0.0279 (6)	0.0379 (7)	−0.0077 (6)	−0.0185 (6)	−0.0002 (5)
C13	0.0398 (7)	0.0373 (7)	0.0596 (9)	0.0001 (5)	−0.0188 (6)	−0.0012 (6)
C14	0.0319 (6)	0.0319 (6)	0.0466 (7)	−0.0050 (5)	−0.0050 (5)	−0.0044 (5)
C15	0.0867 (12)	0.0447 (8)	0.0335 (7)	−0.0317 (8)	0.0095 (7)	−0.0086 (6)

Geometric parameters (Å, °)

O1—C2	1.3528 (12)	C6—H6C	0.9600
O1—C1	1.4376 (16)	C7—C8	1.5058 (14)
O2—C4	1.3404 (12)	C8—C9	1.5038 (14)
O2—C6	1.4338 (14)	C8—H8A	0.9700
O3—C7	1.2235 (12)	C8—H8B	0.9700
N1—C2	1.3279 (12)	C9—C10	1.3865 (16)

N1—C5	1.3356 (12)	C9—C14	1.3947 (16)
N2—C5	1.3298 (12)	C10—C11	1.3991 (16)
N2—C4	1.3373 (12)	C10—H10	0.9300
N3—C7	1.3734 (13)	C11—C12	1.386 (2)
N3—C5	1.3897 (12)	C11—C15	1.507 (2)
N3—H3N	0.875 (15)	C12—C13	1.384 (2)
C1—H1A	0.9600	C12—H12	0.9300
C1—H1B	0.9600	C13—C14	1.3842 (19)
C1—H1C	0.9600	C13—H13	0.9300
C2—C3	1.3843 (15)	C14—H14	0.9300
C3—C4	1.3839 (15)	C15—H15A	0.9600
C3—H3	0.9300	C15—H15B	0.9600
C6—H6A	0.9600	C15—H15C	0.9600
C6—H6B	0.9600		

C2—O1—C1	116.20 (9)	O3—C7—C8	121.00 (9)
C4—O2—C6	117.71 (8)	N3—C7—C8	120.60 (8)
C2—N1—C5	115.15 (8)	C9—C8—C7	111.97 (8)
C5—N2—C4	114.87 (9)	C9—C8—H8A	109.2
C7—N3—C5	132.24 (9)	C7—C8—H8A	109.2
C7—N3—H3N	114.9 (10)	C9—C8—H8B	109.2
C5—N3—H3N	112.9 (10)	C7—C8—H8B	109.2
O1—C1—H1A	109.5	H8A—C8—H8B	107.9
O1—C1—H1B	109.5	C10—C9—C14	119.05 (10)
H1A—C1—H1B	109.5	C10—C9—C8	120.50 (10)
O1—C1—H1C	109.5	C14—C9—C8	120.45 (10)
H1A—C1—H1C	109.5	C9—C10—C11	121.81 (11)
H1B—C1—H1C	109.5	C9—C10—H10	119.1
N1—C2—O1	118.26 (9)	C11—C10—H10	119.1
N1—C2—C3	124.09 (9)	C12—C11—C10	117.89 (12)
O1—C2—C3	117.65 (9)	C12—C11—C15	121.62 (12)
C4—C3—C2	114.49 (9)	C10—C11—C15	120.48 (13)
C4—C3—H3	122.8	C13—C12—C11	121.00 (11)
C2—C3—H3	122.8	C13—C12—H12	119.5
N2—C4—O2	118.59 (9)	C11—C12—H12	119.5
N2—C4—C3	124.04 (9)	C14—C13—C12	120.53 (13)
O2—C4—C3	117.37 (9)	C14—C13—H13	119.7
N2—C5—N1	127.35 (8)	C12—C13—H13	119.7
N2—C5—N3	120.21 (9)	C13—C14—C9	119.71 (13)
N1—C5—N3	112.44 (8)	C13—C14—H14	120.1
O2—C6—H6A	109.5	C9—C14—H14	120.1
O2—C6—H6B	109.5	C11—C15—H15A	109.5
H6A—C6—H6B	109.5	C11—C15—H15B	109.5
O2—C6—H6C	109.5	H15A—C15—H15B	109.5
H6A—C6—H6C	109.5	C11—C15—H15C	109.5
H6B—C6—H6C	109.5	H15A—C15—H15C	109.5
O3—C7—N3	118.39 (9)	H15B—C15—H15C	109.5

C5—N1—C2—O1	179.26 (8)	C7—N3—C5—N1	−176.03 (10)
C5—N1—C2—C3	0.03 (14)	C5—N3—C7—O3	−177.41 (11)

C1—O1—C2—N1	−3.14 (14)	C5—N3—C7—C8	3.42 (17)
C1—O1—C2—C3	176.14 (9)	O3—C7—C8—C9	−6.82 (15)
N1—C2—C3—C4	1.02 (15)	N3—C7—C8—C9	172.33 (9)
O1—C2—C3—C4	−178.21 (9)	C7—C8—C9—C10	−101.24 (11)
C5—N2—C4—O2	−179.18 (9)	C7—C8—C9—C14	79.42 (13)
C5—N2—C4—C3	0.40 (14)	C14—C9—C10—C11	0.61 (16)
C6—O2—C4—N2	5.94 (15)	C8—C9—C10—C11	−178.73 (10)
C6—O2—C4—C3	−173.67 (10)	C9—C10—C11—C12	−0.16 (17)
C2—C3—C4—N2	−1.26 (15)	C9—C10—C11—C15	178.87 (11)
C2—C3—C4—O2	178.33 (9)	C10—C11—C12—C13	−0.20 (19)
C4—N2—C5—N1	0.87 (14)	C15—C11—C12—C13	−179.23 (13)
C4—N2—C5—N3	179.79 (9)	C11—C12—C13—C14	0.1 (2)
C2—N1—C5—N2	−1.08 (14)	C12—C13—C14—C9	0.4 (2)
C2—N1—C5—N3	179.93 (8)	C10—C9—C14—C13	−0.70 (19)
C7—N3—C5—N2	4.91 (16)	C8—C9—C14—C13	178.65 (12)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3N···O3^{i}	0.875 (15)	1.979 (15)	2.8535 (12)	176.0 (14)
C3—H3···O2^{ii}	0.93	2.52	3.4459 (12)	177.

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

Fig. 1

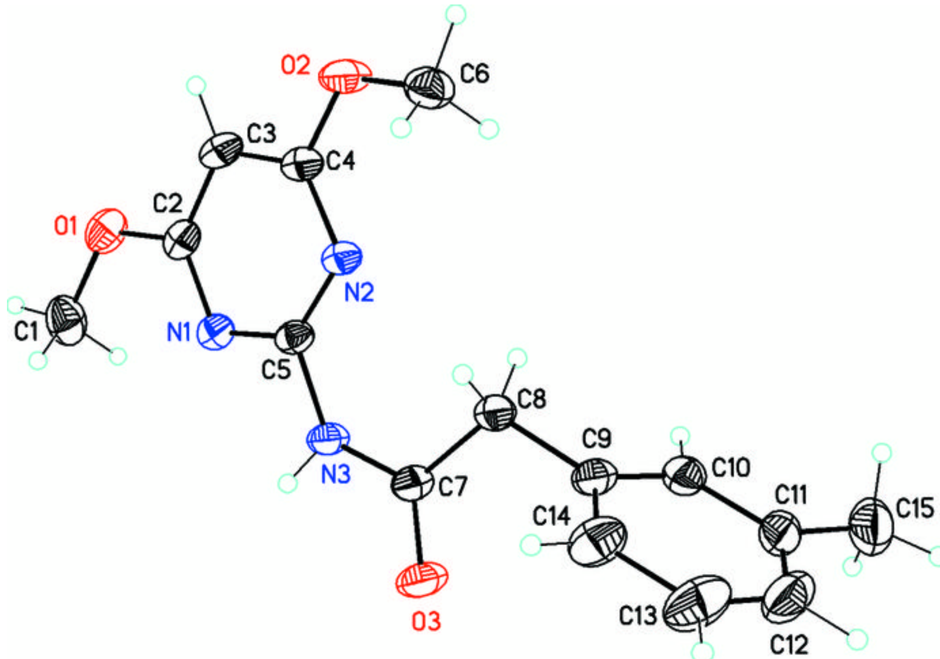

Fig. 2