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N-(2-Bromophenyl)-2-(4,6-dimethoxypyrimidin-2-yloxy)benzylamine

Jun Wu,[a]* Pei-Zhi Zhang,[b] Qing-Sen Yu,[a] Xiu-Rong Hu[c] and Jian-Min Gu[c]

[a]Department of Chemistry, Zhejiang University, Hangzhou, Zhejiang 310027, People's Republic of China, [b]Department of Biological and Chemical Engineering, Zhejiang University of Science and Technology, Hangzhou, Zhejiang 310012, People's Republic of China, and [c]Central Laboratory, Zhejiang University, Hangzhou, Zhejiang 310028, People's Republic of China

Correspondence e-mail: wujunwjwj@sohu.com

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Key indicators

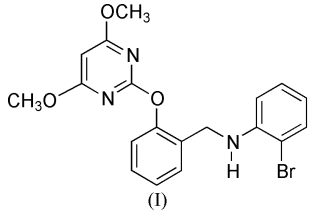
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.006 Å
R factor = 0.048
wR factor = 0.130
Data-to-parameter ratio = 11.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{19}H_{18}BrN_3O_3$, was synthesized by the reaction of 2-methanesulfonyl-4,6-dimethoxypyrimidine and *N*-(2-bromophenyl)-2-hydroxybenzylamine in tetrahydrofuran. There are three different planes in the molecule, each of which is conjugated. The dihedral angles between the pyrimidine plane and the planes of the two phenyl rings are 107.85 (4) and 77.38 (2)°, and the dihedral angle between the planes of the two phenyl rings is 103.15 (3)°.

Comment

4,6-Dimethoxypyrimidines with a phenoxy substituent at the 2-position exhibit marked herbicidal activity (Nezu *et al.*, 1996; Tamaru *et al.*, 1997; Hudson *et al.*, 2002). The new title compound, (I), has shown herbicidal activity against various grass and broadleaf weeds. The present X-ray crystal structure analysis was undertaken in order to improve our understanding of the relationship between structure and activity.



(I)

The molecular structure of (I) is shown in Fig. 1 and selected bond angles are given in Table 1. The bond lengths and angles in the pyrimidine moiety are close to those found in related compounds (Hall *et al.*, 1999; Lin *et al.*, 2001), but the N2—C14—N3 angle [129.7 (3)°] deviates significantly from the normal value. The angles in the two phenyl rings are close

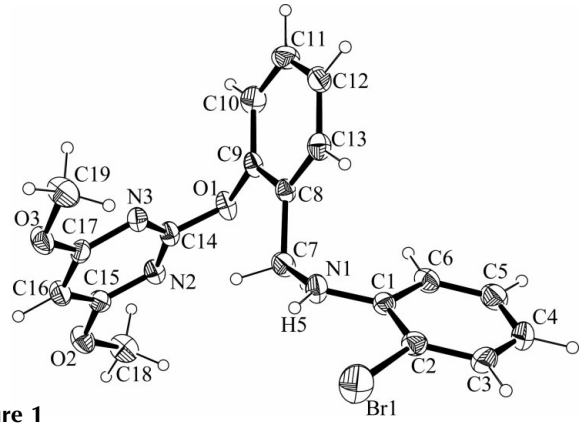


Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 30% probability level and the atom-labeling scheme.

to 120° (Huo *et al.*, 1995), except for the C9—C8—C13 and C2—C1—C6 angles [116.9 (3) and 116.2 (3)°, respectively; Table 1].

The fact that the C9—O1—C14 angle is 119.7 (3)° shows the influence of the pyrimidine and phenyl rings on the ether group (Takashima *et al.*, 1999). The widening of the C1—N1—C7 angle [to 122.5 (3)°] may be due to steric interactions. The N1—C1 bond distance [1.368 (5) Å] is close to that of a C=N double bond, probably as a result of the delocalization of π-electron density between the planes of the two phenyl rings.

There is one intramolecular N—H···Br hydrogen bond (Table 2). The dihedral angles between the pyrimidine plane and the planes of the two phenyl rings are 107.85 (4) and 77.38 (2)°, and the dihedral angle between the planes of the two phenyl rings is 103.15 (3)°

Table 1
Selected bond angles (°).

C9—O1—C14	119.7 (3)	C9—C8—C13	116.9 (3)
C1—N1—C7	122.5 (3)	N2—C14—N3	129.7 (3)
C2—C1—C6	116.2 (3)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H5···Br1	0.94	2.45	3.065 (3)	122

Experimental

To a mixture of *N*-(2-bromophenyl)-2-hydroxybenzylamine (4.29 g, 5.5 mmol) and potassium carbonate (12.96 g, 46.5 mmol) in tetrahydrofuran (THF; 100 ml), a solution of 2-methanesulfonyl-4,6-dimethoxypyrimidine (7.50 g, 17.2 mmol) in THF (40 ml) was added dropwise and the mixture was stirred for 11 h under reflux. The solid was filtered off and the filtrate was left to evaporate at room temperature. After 5 d, a single crystal suitable for X-ray analysis was obtained by recrystallization from ethanol.

Crystal data

$C_{19}H_{18}BrN_3O_3$
M_r = 416.27
Triclinic, $P\overline{1}$
a = 8.7821 (5) Å
b = 10.3347 (6) Å
c = 10.975 (1) Å
α = 104.779 (5)°
β = 92.572 (2)°
γ = 105.331 (2)°
V = 922.1 (1) Å^3
Z = 2
D_x = 1.499 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3573 reflections
θ = 2.1–27.4°
μ = 2.26 mm^{-1}
T = 296.1 K
Platelet, colorless
0.36 × 0.21 × 0.07 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi,1995)
T_{min} = 0.678, T_{max} = 0.854
17 152 measured reflections
4157 independent reflections
2351 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.029
θ_{max} = 27.5°
$h = -9 \rightarrow 11$
$k = -13 \rightarrow 13$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R(F)$ = 0.048
$wR(F^2)$ = 0.130
S = 1.01
2788 reflections
253 parameters
H-atom parameters constrained
$w = 1/[0.002F_o^2 + 1.35\sigma(F_o^2)]/(4F_o^2)$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.97 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

H atoms were placed in calculated positions (C—H = 1.00 Å and N—H = 0.939 Å) and included in the final cycles of refinement as riding atoms.

Data collection: *PROCESS-AUTO* (Molecular Structure Corporation/Rigaku, 2003); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Molecular Structure Corporation/Rigaku, 2003); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *CRYSTALS* (Watkin *et al.*, 1996); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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