

8-Chloro-5-(4-methylpiperazin-1-yl)-11H-pyrido[2,3-b][1,5]benzoxazepine

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Key indicators

Single-crystal X-ray study

T = 293 K

Mean $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$

R factor = 0.040

wR factor = 0.114

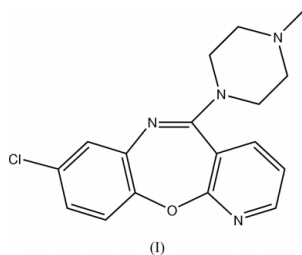
Data-to-parameter ratio = 21.8

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

The crystal structure of the title compound, $\text{C}_{17}\text{H}_{17}\text{ClN}_4\text{O}$, has been undertaken as part of our studies of dopamine receptors. The oxazepine ring has a boat conformation, while the piperazine ring is in a normal chair conformation. The dihedral angle between the two aromatic rings that lie on the same side of the oxazepine moiety is $113.99(7)^\circ$. There is no hydrogen bonding.

Comment

The title compound, (I), also called JL13, was prepared as part of our study of dopamine receptors and related binding sites implicated in schizophrenia (Liégeois, 1992; Liégeois *et al.*, 1993, 1994). It has revealed a very promising antipsychotic profile in several preclinical models (Ellenbroek & Liégeois, 2003). Some crystallographic structures of related compounds have been determined, such as 8-chloro-5-(4-methylpiperazin-1-yl)-11H-pyrido[2,3-b][1,5]benzodiazepine, (II) (Dupont *et al.*, 1996), where an NH group replaces an oxa O atom in the seven-membered ring. In (I), the oxazepine ring has a boat conformation, where the four C atoms of the outer ring junction are almost coplanar; the maximum deviation from their mean plane is $0.021(1) \text{ \AA}$ [(II): $0.034(2) \text{ \AA}$]. The deviation of the 'prow of the boat', *viz.* O5, is $-0.668(1) \text{ \AA}$, and those of N12 and C13 (the 'stern') are $-0.667(1)$ and $-0.762(1) \text{ \AA}$, respectively. The corresponding deviations in (II) are $-0.551(4)$, $-0.668(4)$ and $-0.667(4) \text{ \AA}$, respectively. The distances between the methylpiperazine atom N19 and the centres of the two aromatic rings are $7.758(2)$ and $6.154(2) \text{ \AA}$, respectively [(II): $7.739(4)$ and $6.021(4) \text{ \AA}$]. The dihedral angle between the benzene and pyridine rings is $113.99(7)^\circ$ [(II): $126.4(1)^\circ$]. The cohesion of the crystal is the result of van der Waals interactions (Fig. 2).



Experimental

The title compound was synthesized at the Laboratory of Medicinal Chemistry of Liège (Liégeois *et al.*, 1993). Crystals were obtained by slow evaporation of a methanol solution.

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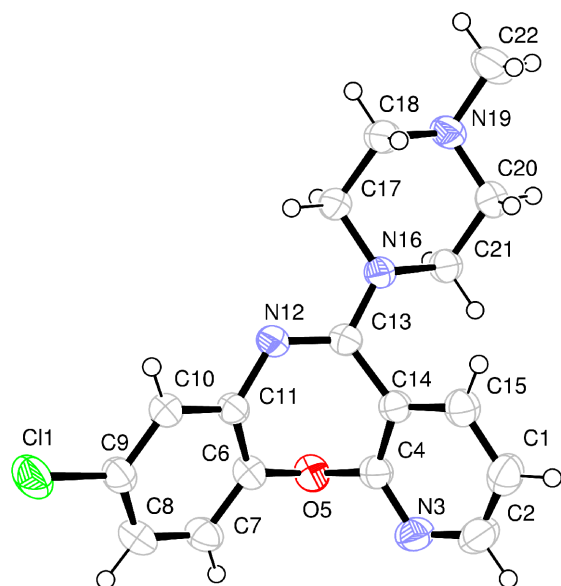


Figure 1
The molecular structure of (I), with the atom-labelling scheme. Displacement ellipsoids are shown at 50% probability levels and H atoms are drawn as small circles of arbitrary radius.

Crystal data

$C_{17}H_{17}ClN_4O$	$D_x = 1.389 \text{ Mg m}^{-3}$
$M_r = 328.80$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 56 reflections
$a = 8.5531(8) \text{ \AA}$	$\theta = 20.2\text{--}22.9^\circ$
$b = 10.6765(8) \text{ \AA}$	$\mu = 0.25 \text{ mm}^{-1}$
$c = 17.2457(12) \text{ \AA}$	$T = 293(2) \text{ K}$
$\beta = 93.347(10)^\circ$	Prism, colourless
$V = 1572.1(2) \text{ \AA}^3$	$0.80 \times 0.57 \times 0.49 \text{ mm}$
$Z = 4$	

Data collection

Stoe–Siemens AED four-circle diffractometer	$R_{\text{int}} = 0.024$
ω scans	$\theta_{\text{max}} = 30.0^\circ$
Absorption correction: ψ scan (EMPIR; Stoe & Cie, 1987)	$h = 0 \rightarrow 12$
$T_{\text{min}} = 0.823$, $T_{\text{max}} = 0.886$	$k = 0 \rightarrow 15$
4860 measured reflections	$l = -24 \rightarrow 24$
4581 independent reflections	2 standard reflections
2865 reflections with $I > 2\sigma(I)$	frequency: 60 min
	intensity decay: 6%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.1871P]$
$R[F^2 > 2\sigma(F^2)] = 0.040$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.114$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.23 \text{ e \AA}^{-3}$
4581 reflections	$\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
210 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.0278 (18)

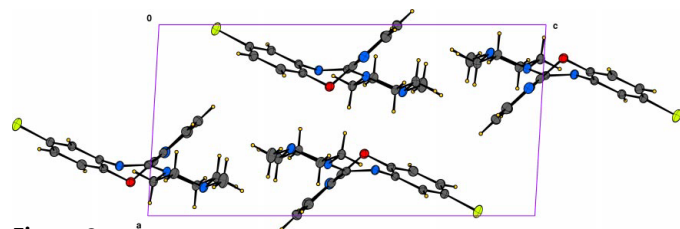


Figure 2
CAMERON (Watkin *et al.*, 1996) view of the packing of (I).

Table 1

Selected geometric parameters (\AA , $^\circ$).

C2–N3	1.335 (2)	C9–C11	1.7403 (15)
N3–C4	1.3153 (19)	C11–N12	1.3972 (16)
C4–O5	1.3867 (17)	N12–C13	1.2986 (16)
O5–C6	1.3971 (16)	C13–N16	1.3667 (17)
C4–N3–C2	116.14 (14)	N12–C13–C14	124.05 (12)
C13–N12–C11	121.94 (12)	C17–N16–C21	111.32 (11)
N12–C13–N16	118.90 (12)	C20–N19–C18	109.64 (11)
N3–C4–O5–C6	109.53 (13)	C11–N12–C13–C14	−8.9 (2)
C14–C4–O5–C6	−70.71 (15)	N12–C13–C14–C4	47.45 (19)
C4–O5–C6–C7	−114.19 (14)	N16–C13–C14–C4	−139.48 (13)
C4–O5–C6–C11	66.68 (16)	C14–C13–N16–C17	−174.80 (12)
O5–C6–C11–N12	6.5 (2)	N12–C13–N16–C21	−149.35 (13)
C6–C11–N12–C13	−39.5 (2)		

H atoms were constrained as riding atoms, with C–H = 0.93–0.97 \AA and with isotropic displacement parameters fixed at $1.2U_{\text{eq}}$ of the parent atom ($1.5U_{\text{eq}}$ for methyl H atoms).

Data collection: *DIF4* (Stoe & Cie, 1987); cell refinement: *DIF4*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

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8-Chloro-5-(4-methylpiperazin-1-yl)-11H-pyrido[2,3-*b*][1,5]benzoxazepine. Erratum**Léon Dupont^{a*} and
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In the paper by Dupont & Liégeois [*Acta Cryst.* (2003), E59, o1962–o1963.], there is an error in the chemical name given in the title. The correct title is '8-Chloro-5-(4-methylpiperazin-1-yl)pyrido[2,3-*b*][1,5]benzoxazepine'.