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# Lansoprazole, an antiulcerative drug[1]

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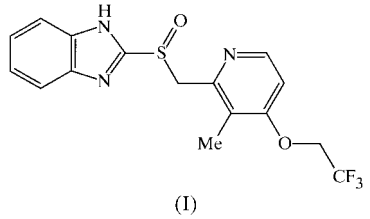
Lansoprazole, 2-({[3-methyl-4-(2,2,2-trifluroethoxy)pyridin-2-yl]methyl}sulfinyl)-1*H*-benzimidazole, $C_{16}H_{14}F_3N_3O_2S$, is an antiulcerative agent. The molecules in the lattice are held together by intermolecular hydrogen bonds between the NH group of benzimidazole and the sulfinyl O atom.

## Comment

The molecule of lansoprazole, (I), does not takes an extended form as found in omeprazole (Ohishi *et al.*, 1989). The torsion angle C7—S1—C8—C9 of −96.0 (2)° contrasts with its value of 179° in omeprazole. This conformation facilitates intramolecular N—H···N hydrogen bonding [N2···N3 = 3.132 (2) Å, H···N3 = 2.49 Å and N2—H···N3 = 139°] between the benzimidazole and pyridine rings. This hydrogen-bond interaction was not found in omeprazole. The dihedral angle between the benzimidazole and pyridine rings is 4.96°, whereas it is 30° in omeprazole. The two molecules which are related by twofold screw axis form an intermolecular N—H···O hydrogen bond [N2···O2($-x$, $y-\frac{1}{2}$, $-z+\frac{1}{2}$) = 2.835 (2) Å, H···O = 2.31 Å and N—H···O = 125°]. This results in a chain of molecules along the *b* direction, while omeprazole forms a cyclic dimer about a centre of symmetry. Stacking interaction between the aromatic rings with a spacing of 3.6 Å confers further stability to the lattice. The average interplanar spacing between pyridine and benzimidazole is 3.4 Å in lansoprazole, while it is 4.13 Å in omeprazole.




(I)

## Experimental

Lansaprazole was prepared according to the method of Prous & Castaner (1989). Crystals suitable for X-ray diffraction were grown from a solution in acetonitrile.

*Crystal data*

$C_{16}H_{14}F_3N_3O_2S$
$M_r$ = 369.36
Monoclinic, $P2_1/c$
$a$ = 15.870 (1) Å
$b$ = 7.3481 (8) Å
$c$ = 14.262 (1) Å
$\beta$ = 102.032 (5)°
$V$ = 1626.7 (2) Å$^3$
$Z$ = 4
$D_x$ = 1.508 Mg m$^{-3}$
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta$ = 32.5–48.2°
$\mu$ = 2.223 mm$^{-1}$
$T$ = 298.2 K
Block, colourless
0.50 × 0.30 × 0.30 mm

*Data collection*

Rigaku AFC-7*S* diffractometer
$\omega$–2$\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.365, $T_{max}$ = 0.513
3347 measured reflections
2961 independent reflections
2853 reflections with $I > 0.1\sigma(I)$
$R_{int}$ = 0.021
$\theta_{max}$ = 70.08°
$h = -19 \rightarrow 18$
$k = -8 \rightarrow 0$
$l = 0 \rightarrow 16$
3 standard reflections
every 150 reflections
intensity decay: 0.06%

*Refinement*

Refinement on $F$
$R$ = 0.047
$wR$ = 0.077
$S$ = 1.939
2853 reflections
231 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o) + 0.00016|F_o|^2]$
$(\Delta/\sigma)_{max}$ = 0.0004
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.38 e Å$^{-3}$
Extinction correction: Zachariasen (1967)
Extinction coefficient: 6 (1) × 10$^{-6}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| S1—O2 | 1.493 (2) | C1—C2 | 1.400 (3) |
| S1—C7 | 1.787 (2) | C1—C6 | 1.389 (3) |
| S1—C8 | 1.845 (2) | C2—C3 | 1.376 (4) |
| F1—C15 | 1.325 (4) | C3—C4 | 1.394 (4) |
| F2—C15 | 1.317 (4) | C4—C5 | 1.367 (4) |
| F3—C15 | 1.326 (3) | C5—C6 | 1.401 (3) |
| O1—C11 | 1.369 (2) | C8—C9 | 1.495 (2) |
| O1—C14 | 1.411 (3) | C9—C10 | 1.394 (2) |
| N1—C6 | 1.391 (3) | C10—C11 | 1.395 (3) |
| N1—C7 | 1.304 (2) | C10—C16 | 1.503 (3) |
| N2—C1 | 1.371 (2) | C11—C12 | 1.378 (3) |
| N2—C7 | 1.345 (3) | C12—C13 | 1.385 (3) |
| N3—C9 | 1.344 (2) | C14—C15 | 1.481 (4) |
| N3—C13 | 1.325 (3) | | |
| O2—S1—C7 | 107.10 (9) | C2—C3—C4 | 122.1 (2) |
| O2—S1—C8 | 106.88 (9) | C3—C4—C5 | 121.6 (2) |
| C7—S1—C8 | 99.11 (9) | C4—C5—C6 | 117.7 (2) |
| C11—O1—C14 | 117.3 (2) | N1—C6—C1 | 110.2 (2) |
| C6—N1—C7 | 103.0 (2) | N1—C6—C5 | 129.7 (2) |
| C1—N2—C7 | 105.7 (2) | C1—C6—C5 | 120.1 (2) |
| C9—N3—C13 | 117.1 (2) | S1—C7—N1 | 120.1 (1) |
| N2—C1—C2 | 132.0 (2) | S1—C7—N2 | 124.5 (1) |
| N2—C1—C6 | 105.7 (2) | N1—C7—N2 | 115.4 (2) |
| C2—C1—C6 | 122.3 (2) | S1—C8—C9 | 110.8 (1) |
| C1—C2—C3 | 116.1 (2) | | |

The H atom of the benzimidazole NH group was refined [N—H = 0.79 (3) Å]. All other H atoms were refined as riding on their carrier atoms (C—H = 0.87–1.00 Å).

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993); cell refinement: *MSC/AFC*

[1] Publication No. 136 from DRF.

*Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1995); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

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