of Kálmán *et al.* (1991)]. Instead, a much weaker hydrogen bond is formed alone, along the longest (*c*) axis *via* the screw axis at $\frac{1}{4}$, 0, *z* in which the acceptor is the ether O atom of the lactone ring (Table 5). A similar type of hydrogen bond is formed in uzarigenin (Kálmán *et al.*, 1991) with somewhat better geometry.

The hydrogen-bond network of telocinobufagin (Table 5) is considerably influenced by the presence of a water molecule which, independently from the position of the lactone ring, spoils the isostructuralism with bufalin. The characteristic 'head-to-tail' hydrogen bond is terminated in such a way that O(1) donates to the water molecule which in turn donates to the oxo group of the lactone ring. In addition, the water molecule builds a third hydrogen bond to the 14β-hydroxy moiety. The latter donates its own intermolecular hydrogen bond to the 5β-hydroxy moiety. In contrast to this, in cinobufotalin (Kálmán *et al.*, 1988) the 5β-hydroxy group acts exclusively as a donor in an intramolecular hydrogen bond to the 3β-hydroxy group. This is common with telocinobufagin. To shed light directly on the lactone-ring effect, crystallization of water-free telocinobufagin has been attempted in various ways, but in vain. Even the co-crystallization of telocinobufagin with bufalin was fruitless.

This joint research was sponsored financially in Hungary by the Hungarian Research Fund, Grant No. OTKA 1806, and in Yugoslavia by the Research Foundation of the Socialist Autonomous Province Vojvodina. The authors thank Professor Lj. Golič (Ljubljana) for data collection on telocinobufagin.

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Structure of the Antipsychotic Drug 3-{2-[4-(6-Fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]ethyl}-2,9-dimethyl-4*H*-pyrido[1,2-*a*]pyrimidin-4-one (Ocaperidone)*

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(*Received* 18 *December* 1991; *accepted* 4 *February* 1992)

Abstract. $C_{24}H_{25}FN_4O_2$, $M_r = 420.5$, monoclinic, $P2_1/n$, $a = 19.95$ (1), $b = 9.782$ (5), $c = 22.07$ (1) Å, $\beta = 102.82$ (3)°, $V = 4201$ (3) Å^3, $Z = 8$, $D_m = 1.32$, $D_x = 1.329$ Mg m^{-3}, graphite-monochromated Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å, $\mu = 0.087$ mm^{-1}, $F(000) = 1776$, $T = 293$ K, final $R = 0.071$ for 7404 unique observed reflections with $|F_o| \geq 4\sigma(|F_o|)$. The asymmetric unit contains two independent molecules *A* and *B*. In both molecules the piperidine ring adopts a chair conformation. For molecule *A*, this ring exhibits site-occupation disorder with the two distinct positions of the piperidine ring almost perpendicular to each other. Molecules *A* and *B* are

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* Internal code of Janssen Pharmaceutica: R79598.

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respectively linked by weak C—H···N and C—H···O hydrogen bonds.

Introduction. Ocaperidone, structurally related to risperidone, is a new very active antipsychotic, pharmacologically characterized by equipotent central dopamine D_2 and serotonine 5-HT_2 antagonism.

Experimental. Colourless crystals were obtained by slow evaporation at room temperature from an acetone solution. The sample used for data collection had dimensions 0.42 × 0.30 × 0.19 mm. Density was measured by flotation in *n*-heptane/CCl_4. Weissenberg photographs indicated the crystals to be monoclinic. Space group $P2_1/n$ was established from systematic absences. The crystal was mounted on a Lindemann glass capillary along **b** and data collected using a Stoe & Co. Stadi-4 diffractometer. Cell constants were determined by least-squares refinement of the setting angles of 24 reflections with $15 < 2\theta < 25°$. $\omega/2\theta$ scans were used to collect data to $[(\sin\theta)/\lambda]_{\max} = 0.5946$ Å^{-1}, and for $0 \le h \le 24$, $0 \le k \le 12$, $-26 \le l \le 26$. The intensities of two standard reflections (202, $51\bar{2}$) were monitored every 180 min and showed no significant variations. From the 8126 reflections measured, 7404 were unique observed reflections with $|F_o| \ge 4\sigma(|F_o|)$. Data reduction was performed with a locally modified version of *REDU*4 (Stoe & Co., 1985). Lorentz and polarization corrections were applied. No absorption corrections were applied owing to the small absorption coefficient. Scattering factors for the non-H atoms were obtained from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B) and for H from Stewart, Davidson & Simpson (1965). The structure was solved with *MULTAN*82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982). The *E* map calculated from the solution with the best figure of merit showed 60 of the 67 non-H atoms. The remaining atoms C(20*A*), C(21*A*), N(16*M*), C(17*M*), C(18*M*), C(20*M*) and C(21*M*) were obtained from a subsequent Fourier synthesis. Refinement was on *F* by full-matrix least squares, first with isotropic temperature factors and finally anisotropically, except for the piperidine ring atoms N(16*M*), C(17*M*), C(18*M*), C(20*M*) and C(21*M*). These atoms were refined with isotropic temperature factors only.

Table 1. *Atomic coordinates and equivalent isotropic displacement parameters* (Å^2 × 10^4) *for molecules A and B, with e.s.d.'s in parentheses*

$B_{eq} = \frac{4}{3}\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j$. Atoms N(16*M*), C(17*M*), C(18*M*), C(20*M*) and C(21*M*), which rely on the disordered moiety in molecule *A*, were refined isotropically.

	x	*y*	*z*	B_{eq}
C(1*A*)	0.0051 (4)	−0.0101 (8)	0.1336 (3)	5.6 (2)
C(2*A*)	0.0610 (4)	−0.0417 (7)	0.1884 (3)	3.8 (2)
C(3*A*)	0.0782 (4)	−0.1711 (7)	0.2090 (4)	4.9 (2)
C(4*A*)	0.1300 (4)	−0.1980 (8)	0.2614 (4)	5.3 (2)
C(5*A*)	0.1674 (4)	−0.0941 (7)	0.2905 (3)	4.8 (2)
N(6*A*)	0.1548 (3)	0.0392 (5)	0.2698 (2)	3.7 (1)
C(7*A*)	0.1011 (4)	0.0699 (7)	0.2202 (3)	3.4 (2)
N(8*A*)	0.0855 (3)	0.1963 (5)	0.2026 (2)	3.5 (1)
C(9*A*)	0.1246 (4)	0.2985 (7)	0.2339 (3)	3.6 (2)
C(10*A*)	0.1812 (4)	0.2768 (7)	0.2805 (3)	3.6 (2)
C(11*A*)	0.2000 (4)	0.1445 (8)	0.3015 (3)	4.6 (2)
C(12*A*)	0.1008 (5)	0.4396 (7)	0.2122 (4)	6.1 (2)
O(13*A*)	0.2477 (3)	0.1098 (6)	0.3425 (3)	7.3 (2)
C(14*A*)	0.2282 (4)	0.3892 (8)	0.3123 (3)	4.7 (2)
C(15*A*)	0.2148 (4)	0.4317 (8)	0.3740 (3)	5.2 (2)
N(16*A*)	0.2721 (4)	0.5092 (8)	0.4113 (4)	3.5 (2)
N(16*M*)	0.2484 (8)	0.581 (2)	0.3949 (6)	2.9 (3)
C(17*A*)	0.2699 (6)	0.644 (1)	0.3829 (5)	4.6 (3)
C(17*M*)	0.219 (1)	0.634 (2)	0.4408 (9)	3.8 (5)
C(18*A*)	0.3303 (7)	0.733 (1)	0.4196 (5)	4.9 (3)
C(18*M*)	0.262 (1)	0.765 (2)	0.4720 (8)	2.8 (4)
C(19*A*)	0.3248 (4)	0.7348 (8)	0.4921 (3)	5.0 (2)
C(20*A*)	0.3267 (7)	0.606 (1)	0.5163 (5)	4.7 (3)
C(20*M*)	0.365 (1)	0.646 (2)	0.4520 (9)	3.4 (4)
C(21*A*)	0.2656 (7)	0.517 (1)	0.4762 (5)	5.3 (3)
C(21*M*)	0.3158 (9)	0.522 (2)	0.4234 (8)	2.7 (4)
C(22*A*)	0.3752 (3)	0.8390 (7)	0.5252 (3)	3.6 (2)
N(23*A*)	0.4159 (3)	0.8086 (6)	0.5785 (3)	4.7 (2)
O(24*A*)	0.4584 (3)	0.9260 (5)	0.5987 (2)	4.8 (1)
C(25*A*)	0.4410 (4)	1.0235 (7)	0.5546 (3)	3.6 (2)
C(26*A*)	0.4683 (4)	1.1529 (7)	0.5556 (3)	4.1 (2)
C(27*A*)	0.4405 (4)	1.2305 (8)	0.5060 (3)	4.8 (2)
C(28*A*)	0.3886 (4)	1.1877 (9)	0.4574 (4)	6.2 (2)
C(29*A*)	0.3610 (4)	1.0605 (8)	0.4575 (3)	5.3 (2)
C(30*A*)	0.3890 (4)	0.9757 (7)	0.5070 (3)	3.6 (2)
F(31*A*)	0.4662 (3)	1.3583 (5)	0.5026 (2)	7.2 (1)
C(1*B*)	0.1617 (5)	0.4609 (9)	0.6023 (3)	7.2 (3)
C(2*B*)	0.1194 (4)	0.5123 (8)	0.5431 (3)	4.6 (2)
C(3*B*)	0.1019 (4)	0.6443 (8)	0.5340 (4)	5.6 (2)
C(4*B*)	0.0613 (5)	0.6898 (8)	0.4774 (4)	6.8 (3)
C(5*B*)	0.0391 (4)	0.6024 (7)	0.4310 (4)	5.8 (2)
N(6*B*)	0.0554 (3)	0.4668 (6)	0.4377 (3)	4.0 (1)
C(7*B*)	0.0958 (4)	0.4185 (7)	0.4926 (3)	4.0 (2)
N(8*B*)	0.1130 (3)	0.2888 (6)	0.4999 (3)	4.5 (2)
C(9*B*)	0.0904 (4)	0.2031 (7)	0.4516 (4)	4.6 (2)
C(10*B*)	0.0491 (4)	0.2402 (8)	0.3963 (3)	4.3 (2)
C(11*B*)	0.0305 (4)	0.3803 (8)	0.3863 (3)	4.4 (2)
C(12*B*)	0.1157 (6)	0.0569 (8)	0.4636 (5)	9.8 (3)
O(13*B*)	−0.0051 (3)	0.4281 (6)	0.3394 (2)	6.7 (2)
C(14*B*)	0.0208 (4)	0.1437 (8)	0.3435 (3)	5.4 (2)
C(15*B*)	−0.0528 (4)	0.0961 (8)	0.3448 (3)	4.6 (2)
N(16*B*)	−0.0821 (3)	0.0031 (6)	0.2937 (3)	4.0 (2)
C(17*B*)	−0.1569 (4)	−0.0093 (8)	0.2881 (4)	4.9 (2)
C(18*B*)	−0.1902 (4)	−0.0990 (7)	0.2345 (4)	4.7 (2)
C(19*B*)	−0.1594 (3)	−0.2409 (7)	0.2413 (3)	3.6 (2)
C(20*B*)	−0.0813 (4)	−0.2278 (8)	0.2500 (3)	5.0 (2)
C(21*B*)	−0.0512 (4)	−0.1331 (7)	0.3038 (4)	5.2 (2)
C(22*B*)	−0.1882 (3)	−0.3345 (7)	0.1883 (3)	3.6 (2)
N(23*B*)	−0.2365 (3)	−0.2906 (6)	0.1425 (3)	4.4 (2)
O(24*B*)	−0.2539 (3)	−0.4040 (5)	0.1003 (2)	4.7 (1)
C(25*B*)	−0.2144 (4)	−0.5100 (7)	0.1251 (3)	3.9 (2)
C(26*B*)	−0.2150 (4)	−0.6399 (8)	0.0983 (3)	4.4 (2)
C(27*B*)	−0.1701 (4)	−0.7293 (7)	0.1330 (4)	4.8 (2)
C(28*B*)	−0.1272 (4)	−0.6999 (8)	0.1887 (3)	5.1 (2)
C(29*B*)	−0.1266 (4)	−0.5711 (8)	0.2134 (3)	4.6 (2)
C(30*B*)	−0.1715 (3)	−0.4753 (7)	0.1807 (3)	3.5 (2)
F(31*B*)	−0.1670 (3)	−0.8573 (5)	0.1092 (2)	7.1 (1)

At an intermediate stage in the refinement, difference maps showed maxima in positions consistent with the expected locations of H atoms; in the final round of calculations the H atoms were placed at a riding distance of 0.95 Å and included in the structure-factor calculations with a fixed isotropic temperature factor of *B* equal to 1.33 times the B_{eq} value of the parent atom. The H atoms attached at the piperidine ring of molecule *A* were not determined. Final refinement was on *F* by least-squares methods, refining 579 parameters, $R = 0.071$, $wR = 0.075$ with $w = 4F^2/[\sigma^2(I) + (0.04F^2)^2]$, $S = 2.71$. Largest parameter shift/e.s.d. = 0.06. Minimum and maximum residual electron densities were −0.32 and 0.37 e Å^{-3}. The number of reflections per

Table 2. *Bond lengths* (Å), *bond angles* (°) *and selected torsion angles* (°) *for molecules A and B, with e.s.d.'s in parentheses*

	Molecule *A*	Molecule *B*
C(1)—C(2)	1.484 (9)	1.48 (2)
C(2)—C(3)	1.362 (9)	1.35 (1)
C(2)—C(7)	1.45 (1)	1.45 (2)
C(3)—C(4)	1.39 (2)	1.40 (1)
C(4)—C(5)	1.34 (2)	1.33 (1)
C(5)—N(6)	1.386 (9)	1.367 (9)
N(6)—C(7)	1.385 (8)	1.381 (8)
N(6)—C(11)	1.444 (9)	1.414 (9)
C(7)—N(8)	1.312 (8)	1.315 (9)
N(8)—C(9)	1.359 (8)	1.35 (1)
C(9)—C(10)	1.365 (9)	1.363 (9)
C(9)—C(12)	1.50 (1)	1.52 (1)
C(10)—C(11)	1.40 (1)	1.42 (2)
C(10)—C(14)	1.51 (1)	1.51 (2)
C(11)—O(13)	1.207 (9)	1.212 (8)
C(14)—C(15)	1.50 (2)	1.55 (1)
C(15)—N(16)	1.46 (2)	1.467 (9)
C(15)—N(16*M*)	1.63 (2)	
N(16)—C(17)	1.45 (1)	1.477 (9)
N(16)—C(21)	1.47 (1)	1.463 (9)
N(16*M*)—C(17*M*)	1.38 (3)	
N(16*M*)—C(21*M*)	1.48 (2)	
C(17)—C(18)	1.56 (2)	1.50 (2)
C(17*M*)—C(18*M*)	1.61 (3)	
C(18)—C(19)	1.63 (1)	1.51 (1)
C(18*M*)—C(19)	1.27 (2)	
C(19)—C(20)	1.36 (1)	1.54 (2)
C(19)—C(20*M*)	1.58 (2)	
C(19)—C(22)	1.50 (1)	1.496 (9)
C(20)—C(21)	1.60 (2)	1.52 (2)
C(20*M*)—C(21*M*)	1.60 (3)	
C(22)—N(23)	1.307 (8)	1.306 (9)
C(22)—C(30)	1.45 (2)	1.43 (1)
N(23)—O(24)	1.438 (7)	1.441 (7)
O(24)—C(25)	1.354 (8)	1.343 (8)
C(25)—C(26)	1.38 (1)	1.40 (2)
C(25)—C(30)	1.383 (9)	1.373 (9)
C(26)—C(27)	1.35 (1)	1.36 (1)
C(27)—C(28)	1.38 (2)	1.36 (1)
C(27)—F(31)	1.360 (9)	1.365 (9)
C(28)—C(29)	1.36 (1)	1.37 (2)
C(29)—C(30)	1.39 (1)	1.38 (1)
C(1)—C(2)—C(3)	123.6 (6)	122.7 (8)
C(1)—C(2)—C(7)	118.3 (6)	119.5 (7)
C(3)—C(2)—C(7)	118.1 (6)	117.9 (6)
C(2)—C(3)—C(4)	122.6 (6)	121.2 (7)
C(3)—C(4)—C(5)	119.1 (7)	120.6 (8)
C(4)—C(5)—N(6)	121.0 (6)	120.7 (8)
C(5)—N(6)—C(7)	121.1 (5)	120.3 (6)
C(5)—N(6)—C(11)	117.7 (5)	117.5 (6)
C(7)—N(6)—C(11)	121.3 (5)	122.2 (6)
C(2)—C(7)—N(6)	118.0 (6)	119.2 (6)
C(2)—C(7)—N(8)	120.0 (5)	119.2 (6)
N(6)—C(7)—N(8)	121.9 (6)	121.6 (7)
C(7)—N(8)—C(9)	118.1 (5)	117.9 (6)
N(8)—C(9)—C(10)	123.7 (7)	124.8 (7)
N(8)—C(9)—C(12)	114.2 (6)	113.9 (6)
C(10)—C(9)—C(12)	122.2 (6)	121.3 (7)
C(9)—C(10)—C(11)	120.7 (6)	118.8 (6)
C(9)—C(10)—C(14)	124.1 (6)	125.0 (7)
C(11)—C(10)—C(14)	115.3 (6)	116.3 (6)
N(6)—C(11)—C(10)	114.0 (6)	114.7 (6)
N(6)—C(11)—O(13)	117.8 (6)	119.3 (7)
C(10)—C(11)—O(13)	128.3 (7)	125.9 (7)
C(10)—C(14)—C(15)	113.8 (7)	111.6 (7)
C(14)—C(15)—N(16)	112.3 (7)	113.0 (6)
C(14)—C(15)—N(16*M*)	111.1 (8)	
C(20*M*)—C(19)—C(22)	106.4 (9)	
C(19)—C(20)—C(21)	109.5 (8)	111.3 (7)
C(19)—C(20*M*)—C(21*M*)	108 (1)	
N(16)—C(21)—C(20)	110 (1)	110.8 (6)
N(16*M*)—C(21*M*)—C(20*M*)	107 (1)	
C(15)—N(16)—C(17)	106.3 (7)	109.8 (6)
C(15)—N(16)—C(21)	110.4 (8)	111.5 (5)
C(17)—N(16)—C(21)	111.9 (8)	108.7 (6)
C(15)—N(16*M*)—C(17*M*)	109 (1)	
C(15)—N(16*M*)—C(21*M*)	93 (2)	
C(17*M*)—N(16*M*)—C(21*M*)	109 (1)	
N(16)—C(17)—C(18)	109.6 (8)	112.1 (6)
N(16*M*)—C(17*M*)—C(18*M*)	111 (2)	
C(17)—C(18)—C(19)	107.7 (9)	111.0 (6)
C(17*M*)—C(18*M*)—C(19)	112 (1)	

Table 2 (*cont.*)

	Molecule *A*	Molecule *B*
C(18)—C(19)—C(20)	111.9 (8)	108.4 (6)
C(18)—C(19)—C(22)	107.5 (7)	114.0 (5)
C(18*M*)—C(19)—C(20*M*)	121 (1)	
C(18*M*)—C(19)—C(22)	121 (2)	
C(20)—C(19)—C(22)	118.5 (7)	110.7 (6)
C(19)—C(22)—N(23)	119.9 (6)	119.7 (6)
C(19)—C(22)—C(30)	130.0 (6)	128.3 (5)
N(23)—C(22)—C(30)	110.0 (6)	112.1 (6)
C(22)—N(23)—O(24)	107.7 (5)	106.1 (5)
N(23)—O(24)—C(25)	107.4 (5)	107.2 (5)
O(24)—C(25)—C(26)	126.8 (6)	125.3 (6)
O(24)—C(25)—C(30)	109.7 (6)	111.5 (7)
C(26)—C(25)—C(30)	123.5 (7)	123.3 (6)
C(25)—C(26)—C(27)	114.5 (7)	113.7 (6)
C(26)—C(27)—C(28)	124.4 (7)	125.1 (8)
C(26)—C(27)—F(31)	118.0 (6)	116.9 (6)
C(28)—C(27)—F(31)	117.7 (7)	117.9 (6)
C(27)—C(28)—C(29)	120.6 (7)	120.0 (7)
C(28)—C(29)—C(30)	117.1 (6)	117.8 (6)
C(22)—C(30)—C(25)	105.1 (5)	103.2 (6)
C(22)—C(30)—C(29)	135.0 (6)	136.7 (6)
C(25)—C(30)—C(29)	119.9 (7)	120.1 (7)
C(1)—C(2)—C(3)—C(4)	−178.7 (7)	−179.6 (8)
C(5)—N(6)—C(11)—O(13)	3.0 (10)	−1.7 (10)
C(9)—C(10)—C(14)—C(15)	99.9 (8)	96.0 (9)
C(10)—C(14)—C(15)—N(16)	163.2 (6)	179.4 (6)
C(10)—C(14)—C(15)—N(16*M*)	−161.8 (7)	
C(14)—C(15)—N(16)—C(21)	−165.0 (7)	74.2 (7)
C(14)—C(15)—N(16*M*)—C(21*M*)	−37.6 (29)	
C(17)—C(18)—C(19)—C(22)	−170.6 (7)	−177.8 (6)
C(17*M*)—C(18*M*)—C(19)—C(22)	−177.9 (10)	
C(22)—C(19)—C(20)—C(21)	176.2 (8)	−179.9 (6)
C(22)—C(19)—C(20*M*)—C(21*M*)	172.6 (10)	
C(20)—C(19)—C(22)—N(23)	−5.2 (12)	−123.6 (7)
C(20*M*)—C(19)—C(22)—N(23)	−86.4 (10)	
C(18)—C(19)—C(22)—N(23)	133.3 (8)	−1.1 (9)
C(18*M*)—C(19)—C(22)—N(23)	130.3 (12)	
O(24)—C(25)—C(26)—C(27)	−178.7 (7)	−179.8 (7)

refined variable was 3704/578 = 6.4. All calculations were performed on a Digital PDP-11/73 microcomputer using *SDP* (B. A. Frenz & Associates, Inc., 1985) and *PARST* (Nardelli, 1983).

Discussion. Final atomic coordinates and equivalent isotropic displacement parameters are listed in Table 1. Main bond lengths, bond angles and selected torsion angles are given in Table 2.*

The asymmetric unit contains two molecules *A* and *B*. The piperidine ring of molecule *A* shows positional disorder and has been refined in two positions (*A* and *M*). A *PLUTO* plot (Motherwell & Clegg, 1978) of molecule *A*, with the two positionally disordered piperidine rings, is shown in Fig. 1. Molecule *B*, with the numbering scheme adopted, is shown in Fig. 2. A stereoscopic view of the molecular packing viewed down **b** is given in Fig. 3.

The piperidine ring atoms N(16*A*), C(17*A*), C(18*A*), C(20*A*) and C(21*A*) showed an occupancy factor of 0.65 and were refined anisotropically. The other positions N(16*M*), C(17*M*), C(18*M*), C(20*M*)

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* Lists of structure factors, anisotropic thermal parameters, bond lengths and angles involving H atoms, H-atom parameters, and least-squares data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55142 (34 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

and C(21*M*) were refined isotropically and exhibited a multiplicity factor of 0.35. The dihedral angle between the mean planes defined by the piperidine ring atoms with occupancies of 0.65 and 0.35 respectively measures 92.0 (5)°. As a result of this site-occupation disorder the piperidine ring of molecule *A* shows ring distortion.

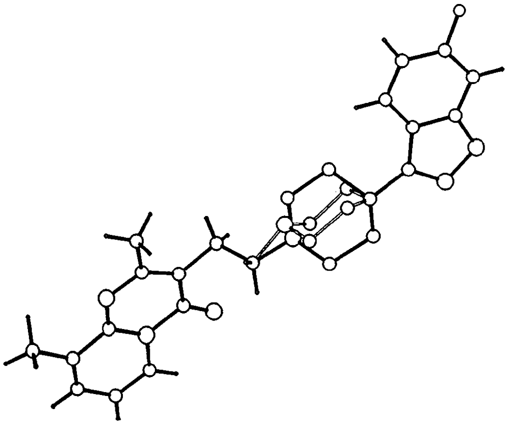

Fig. 1. A *PLUTO* plot (Motherwell & Clegg, 1978) of molecule *A*, with the two positions of the piperidine ring.

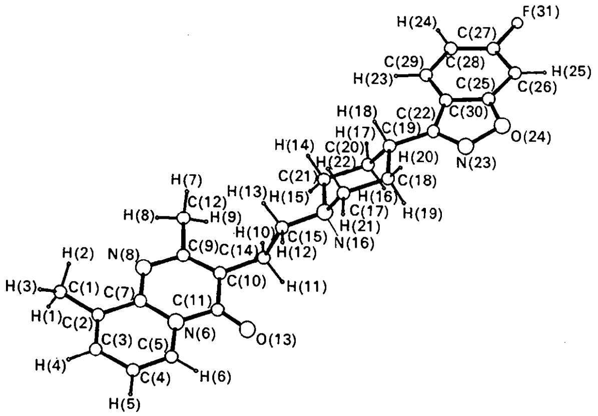

Fig. 2. A *PLUTO* plot (Motherwell & Clegg, 1978) of molecule *B* showing the numbering scheme.

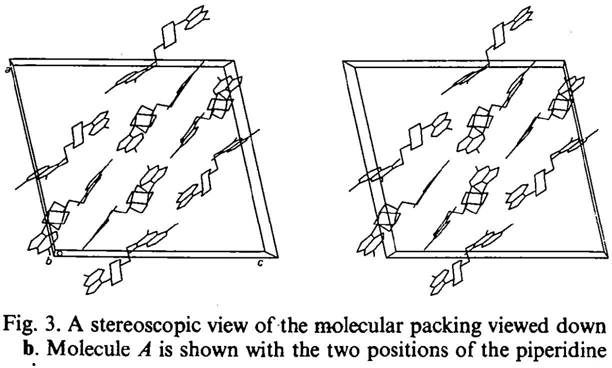

Fig. 3. A stereoscopic view of the molecular packing viewed down **b**. Molecule *A* is shown with the two positions of the piperidine ring.

The groups of atoms of both pyridopyrimidine rings and both benzisoxazole rings are only slightly displaced from the least-squares plane. Maximum out of plane deviations are 0.030 (8) Å for C(3*A*) and −0.029 (7) Å for C(9*A*).

Atoms C(1*A*), C(1*B*), O(13*A*) and O(13*B*) show out of plane deviations of 0.011 (8), −0.016 (10), 0.040 (6) and 0.001 (6) Å respectively and are coplanar with the pyridopyrimidine ring system. Atoms F(31*A*) and F(31*B*) with out of plane deviations of 0.040 (5) and 0.037 (5) Å are coplanar with the benzisoxazole ring.

For the piperidine ring of molecule *A* we calculated, following the method of Cremer & Pople (1975), a phase angle $\theta_2 = 179\,(1)$ and $\varphi_2 = -157\,(141)°$, indicating a chair conformation, and a puckering amplitude $Q = 0.593\,(11)$ Å for the sequence N(16*A*)—C(17*A*)—C(18*A*)—C(19*A*)—C(20*A*)—C(21*A*). For the sequence N(16*B*)—C(17*B*)—C(18*B*)—C(19*B*)—C(20*B*)—C(21*B*) in molecule *B*, $\theta_2 = 2.3\,(7)$, $\varphi_2 = -12\,(18)°$ and $Q = 0.584\,(7)$ Å were obtained.

Intermolecular hydrogen bonds (Taylor & Kennard, 1982) are formed between the pyridopyrimidine H atom H(1*A*) and the benzisoxazole N atom N(23*A*): H(1*A*)···N(23$A^{\rm i}$)* = 2.57 (1) Å. Hydrogen bonds are also found between the benzisoxazole H(23*B*) atom and the pyridopyrimidine O atom O(13*B*): H(23*B*)···O(13$B^{\rm ii}$) = 2.36 (1) Å. No other contacts shorter than the sums of the van der Waals radii were observed.

The authors wish to thank the Janssen Research Foundation (Janssen Pharmaceutica, B-2340 Beerse, Belgium) for providing the R79598 sample.

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* Symmetry code: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$; (ii) $x, y - 1, z$.

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