C(5α)—C(5)—C(4)	129.1 (4)	C(5β)—C(5α)—C(5)	113.6 (4)
O(5γ)—C(5β)—C(5α)	113.3 (4)	C(3,5′)—N(3)—C(2)	120.0 (3)
C(3,5′)—N(3)—C(4)	123.9 (4)	N(3′)—C(2′)—N(1′)	126.3 (4)
C(4′)—N(3′)—C(2′)	117.8 (4)	C(4′)—C(5′)—C(3,5′)	121.0 (4)
C(5′)—C(3,5′)—N(3)	112.0 (4)	C(5′)—C(4′)—N(3′)	120.5 (4)
C(5′)—C(6′)—N(1′)	124.1 (4)	C(6′)—N(1′)—C(2′)	115.6 (4)
C(6′)—C(5′)—C(3,5′)	123.1 (4)	C(6′)—C(5′)—C(4′)	115.7 (4)
C(2′α)—C(2′)—N(1′)	116.5 (4)	C(2′α)—C(2′)—N(3′)	117.2 (4)
N(4′α)—C(4′)—N(3′)	117.2 (4)	N(4′α)—C(4′)—C(5′)	122.3 (4)
C(1*A*)—C(2*A*)—C(3*A*)	122. (2)	O(*A*)—C(2*A*)—C(1*A*)	118 (2)
O(*A*)—C(2*A*)—C(3*A*)	120 (2)		

Table 3. *Hydrogen-bonding geometry* (Å, °)

D—H···*A*	H···*A*	*D*···*A*	*D*—H···*A*
N(4′α)—H(1)···O(5γ^{i})	1.97 (5)	2.915 (5)	173 (5)
N(4′α)—H(2)···N($3'^{ii}$)	2.26 (5)	3.117 (5)	165 (5)
O(5γ)—H···N($1'^{iii}$)	1.95 (5)	2.814 (4)	176 (5)

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

The structure was solved by direct methods and refined by full-matrix least squares using *SHELX*76 (Sheldrick, 1976). A difference map after anisotropic refinement of the TTT molecule revealed the peaks for all H atoms of TTT and additional prominent peaks near the inversion centre at $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. These peaks were identified, with difficulty, as the disordered acetone solvate, based on the interpretation of the geometrical relationships of the peaks, the NMR spectra and the elemental analysis data of the crystal. In the final cycle of refinement, each H atom was assigned a fixed isotropic displacement parameter 1.3 times greater than the isotropic equivalent of the atom to which it is attached. H atoms in the acetone molecule could not be located and were not included in the structure-factor calculations.

This work was supported by a grant from the Korea Science and Engineering Foundation.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and bond distances and angles involving H atoms have been deposited with the IUCr (Reference: HR1001). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Cooks, R. G. & Sykes, P. (1968). *J. Chem. Soc.* pp. 2871–2876.
Cramer, R. E., Maynard, R. B. & Ibers, J. A. (1981). *J. Am. Chem. Soc.* **103**, 76–81.
Dyda, F., Furey, W., Swaminathan, S., Sax, M., Farrenkopf, B. & Jordan, F. (1993). *Biochemistry*, **32**, 6165–6170.
Gutowski, J. A. & Lienhard, G. E. (1976). *J. Biol. Chem.* **251**, 2863–2866.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Kluger, R., Gish, G. & Kauffman, G. (1984). *J. Biol. Chem.* **259**, 8960–8965.
Kraut, J. & Reed, H. J. (1962). *Acta Cryst.* **15**, 747–757.
Kuo, D. J. & Jordan, F. (1983). *J. Biol. Chem.* **258**, 13415–13417.
Lindqvist, Y., Schneider, G., Ermler, U. & Sundström, M. (1992). *EMBO J.* **11**, 2372–2379.
Muller, Y. A. & Schulz, G. E. (1993). *Science*, **259**, 965–967.
Pletcher, J., Sax, M., Blank, G. & Wood, M. (1977). *J. Am. Chem. Soc.* **99**, 1396–1403.
Rochester, J., Berg, U., Pierrot, M. & Sandström, J. (1987). *J. Am. Chem. Soc.* **109**, 492–507.
Saenger, V. W. & Suck, D. (1971). *Acta Cryst.* B**27**, 1178–1186.
Sax, M., Pulsinelli, P. & Pletcher, J. (1974). *J. Am. Chem. Soc.* **96**, 155–165.
Schellenberger, A. (1967). *Angew. Chem. Int. Ed. Engl.* **6**, 1024–1035.
Schmidt, M. W., Truong, P. N. & Gordon, M. S. (1987). *J. Am. Chem. Soc.* **109**, 5217–5227.
Sheldrick, G. M. (1976). *SHELX76. Program for Crystal Structure Determination.* Univ. of Cambridge, England.
Shin, W. & Kim, Y. C. (1986). *J. Am. Chem. Soc.* **108**, 7078–7082.
Shin, W. & Lah, M. S. (1987). *Acta Cryst.* C**43**, 125–129.
Shin, W., Oh, D. K., Chae, C. H. & Yoon, T. S. (1993). *J. Am. Chem. Soc.* **115**, 12238–12250.
Shin, W., Pletcher, J. & Sax, M. (1979). *J. Am. Chem. Soc.* **101**, 4365–4371.

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The Novel GABA$_A$ Receptor Ligand NNC 14-0764: 5-(3-Cyclopropyl-1,2,4-oxadiazol-5-yl)-2,3-dihydrodiimidazo[1,5-*a*:1′,2′-*c*]-quinazoline

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Abstract

The crystal and molecular structure of the title compound, $C_{17}H_{14}N_6O$, has been determined. The two molecules in the asymmetric unit have very similar geometrical features, the major difference being in the overall convex or concave shape of the molecular surface. As a consequence, although as expected, the cyclopropyl rings are approximately perpendicular to the general molecular plane; the three C atoms of the cyclopropyl groups are distributed quite differently above and below the general molecular plane in the two molecules. Consequences of this effect for theoretical consideration of drug activity are discussed.

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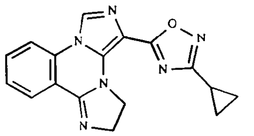
Comment

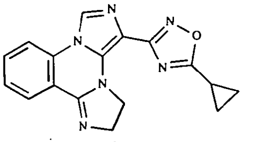
The title compound (I*a*) is a member of a novel series of compounds which exhibit strong affinity for the GABA_A receptor (Im, Im, Pregenzer, Petke, Hamilton, Carter, von Voigtlander, Hansen & Kristiansen, 1992). These drugs act upon the central nervous system, and although they are similar in chemical structure they have remarkably different pharmacological properties (Im *et al.*, 1992). The objectives of the present study were to confirm the molecular structure of (I*a*) and to provide accurate geometrical parameters for future quantitative structure–activity studies of these compounds.

NNC 14-0764



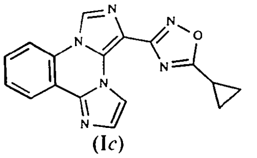
(I*a*)

NNC 14-0763



(I*b*)

NNC 14-0765



(I*c*)

Fig. 1 shows a view of molecule 1 perpendicular to the least-squares plane and the numbering scheme used in the X-ray analysis. The assignment of the atom labels C2*B* and C3*B* in the cyclopropyl rings of the two molecules is arbitrary, and the actual choice of labelling has been made in order to maximize compatibility between the descriptions of molecular geometry given below.

The bond lengths for the two molecules in the asymmetric unit agree within acceptable limits, and confirm, essentially, the assigned structure of (I*a*). Of the small variations in the lengths of bonds of the same type observed in these two structures, the most significant are for the N=C bonds N1=C16, N7=C8, N1*A*=C5*A* and N4*A*=C3*A*, with values ranging from 1.274 (2) to 1.301 (2) Å, the larger values being for the linked oxadiazole ring *A* (Fig. 1) external to the fused heterocyclic ring system *CDEF*. There are no unusual bond angles. Significant variations in the external ring angles of the two molecules are noted in Fig. 1 and in Table 2; the torsion angles in the two molecules are very similar. The differences in conformation can be illustrated by comparing the dihedral angles in different parts of the two molecules. In both molecules, the diimidazoquinazoline moieties (rings *C*, *D*, *E* and *F*) and the oxadiazole rings (*A*) are essentially planar. The equations for the relevant least-squares planes and the deviations of atom positions from them are given in Table 3. From these data it can be seen that the dihedral angles between the cyclopropyl ring *B* and the oxadiazole ring *A* differ by about 3.7 (2)° between molecules 1 and 2 but with atom C2*B* above, C3*B* below and C1*B* lying approximately in the oxadiazole ring plane in both molecules. As a consequence of differences between the diimidazoquinazoline plane and oxadiazole plane in the two molecules, however, atom C2*B* is above, C3*B* below and C1*B* lies approximately in the plane of the diimidazoquinazoline group in molecule 1, whereas in molecule 2, atoms C1*B*′ and C3*B*′ are both below and C2*B*′ lies approximately in this plane. The consequences of these differences in molecular conformation can be seen in Fig. 2, which indicates a dramatic overall difference in the curvature of the two molecules.

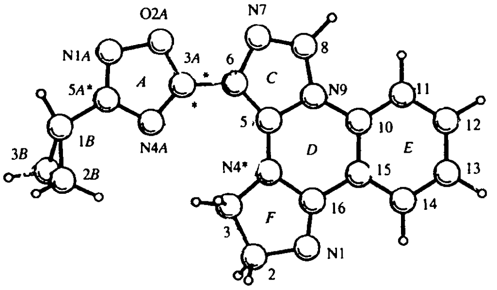


Fig. 1. A view of molecule 1 perpendicular to the least-squares plane, showing the atom-numbering scheme used in the X-ray analysis (atom numbers in molecule 1 are primed). An asterisk (*) denotes external ring angles differing by $>3\sigma$ between molecules 1 and 2.

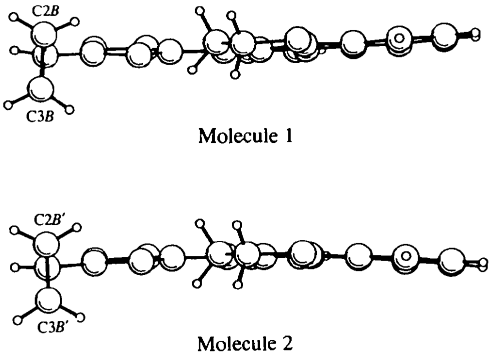


Fig. 2. Molecular profiles showing the opposing curvature of the two molecules in the asymmetric unit, where the atoms labelled *B* are part of the cyclopropyl rings.

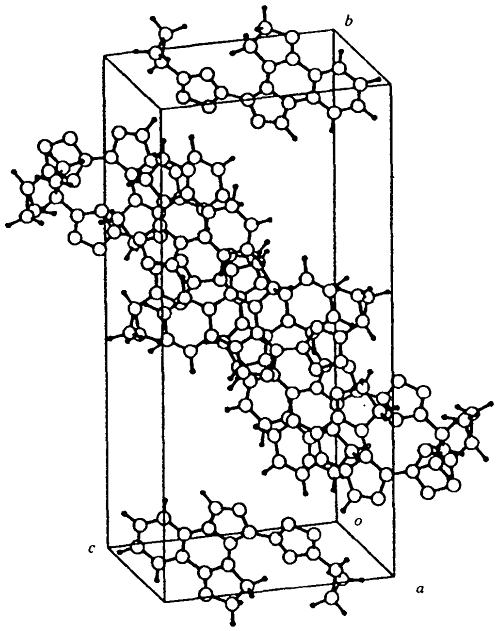


Fig. 3. A view of the crystal packing showing the stacking of the ring systems.

The molecules form van der Waals stacks (Fig. 3) in the crystal structure, there being no other types of intermolecular forces present.

Previous studies (Im *et al.*, 1992) indicated that the energetics of analogues in the present series of diimidazoquinazolines are based on the relative orientations of the cyclopropyloxadiazole group and the diimidazoquinazoline ring system treated as two separate units. The present analysis fortuitously affords two independent conformers of one member of the series, and suggests that in view of the differences observed in the orientation of the cyclopropyl group the approach should in fact proceed *via* consideration of the cyclopropyl group, the oxadiazole ring and the diimidazoquinazoline group, and their relative orientations.

Experimental

Crystal data

$C_{17}H_{14}N_6O$
$M_r = 318.34$
Monoclinic
$P2_1/a$
$a = 8.693$ (3) Å
$b = 26.794$ (7) Å
$c = 12.534$ (5) Å
$\beta = 93.08$ (3)°
$V = 2915.0$ Å^3
$Z = 8$
$D_x = 1.451$ Mg m^{-3}

Cu $K\alpha$ radiation
$\lambda = 1.54178$ Å
Cell parameters from 25 reflections
$\theta = 20$–25°
$\mu = 0.790$ mm^{-1}
$T = 293$ K
Needle
0.6 × 0.3 × 0.3 mm
Colourless
Crystal source: Novo Nordisk

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: none
11 733 measured reflections
5833 independent reflections
5149 observed reflections [$I > 2\sigma(I)$]
$R_{\rm int} = 0.0287$

$\theta_{\rm max} = 73°$
$h = -10 \rightarrow 9$
$k = -15 \rightarrow 33$
$l = -15 \rightarrow 15$
3 standard reflections monitored every 100 reflections
intensity decay: <10%

Refinement

Refinement on F^2
$R[I > 2\sigma(I)] = 0.0365$
$wR(F^2) = 0.1053$
$S = 1.000$
5833 reflections
462 parameters
Only H-atom U's refined
$w = 1/\sigma^2(F_o^2)$
$(\Delta/\sigma)_{\rm max} = -0.001$ (for the z coordinate of N9)

$\Delta\rho_{\rm max} = 0.213$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.186$ e Å^{-3}
Extinction correction: *SHELXL*92 (Sheldrick, 1992)
Extinction coefficient: 0.002 (1)
Atomic scattering factors from *SHELXL*92 (Sheldrick, 1992)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Molecule 1				
N1	0.5819 (2)	0.6072 (1)	0.5922 (1)	0.055 (1)
C2	0.6491 (2)	0.6235 (1)	0.4927 (1)	0.053 (1)
C3	0.7407 (2)	0.5793 (1)	0.4512 (1)	0.048 (1)
N4	0.6870 (1)	0.5390 (1)	0.5186 (1)	0.044 (1)
C5	0.7352 (2)	0.4904 (1)	0.5211 (1)	0.041 (1)
C6	0.8247 (2)	0.4603 (1)	0.4598 (1)	0.044 (1)
N7	0.8311 (2)	0.4125 (1)	0.5038 (1)	0.051 (1)
C8	0.7495 (2)	0.4139 (1)	0.5867 (1)	0.050 (1)
N9	0.6874 (2)	0.4606 (1)	0.6025 (1)	0.044 (1)
C10	0.5983 (1)	0.4777 (1)	0.6858 (1)	0.044 (1)
C11	0.5566 (2)	0.4462 (1)	0.7670 (1)	0.052 (1)
C12	0.4745 (2)	0.4650 (1)	0.8490 (1)	0.058 (1)
C13	0.4314 (2)	0.5148 (1)	0.8493 (1)	0.061 (1)
C14	0.4704 (2)	0.5462 (1)	0.7681 (1)	0.054 (1)
C15	0.5558 (2)	0.5280 (1)	0.6856 (1)	0.045 (1)
C16	0.6054 (2)	0.5603 (1)	0.6002 (1)	0.044 (1)
N1*A*	1.0633 (2)	0.4509 (1)	0.2388 (1)	0.061 (1)
O2*A*	0.9935 (1)	0.4329 (1)	0.3315 (1)	0.059 (1)
C3*A*	0.9056 (2)	0.4701 (1)	0.3652 (1)	0.043 (1)
N4*A*	0.9109 (1)	0.5098 (1)	0.3056 (1)	0.049 (1)
C5*A*	1.0091 (2)	0.4959 (1)	0.2287 (1)	0.047 (1)
C1*B*	1.0532 (2)	0.5290 (1)	0.1426 (1)	0.056 (1)
C2*B*	1.0571 (2)	0.5839 (1)	0.1627 (2)	0.065 (1)
C3*B*	0.9358 (2)	0.5628 (1)	0.0895 (2)	0.073 (1)
Molecule 2				
N1′	0.7234 (2)	0.3444 (1)	0.1735 (1)	0.054 (1)
C2′	0.8064 (2)	0.3625 (1)	0.0825 (1)	0.058 (1)
C3′	0.8706 (2)	0.3167 (1)	0.0257 (1)	0.048 (1)
N4′	0.8070 (1)	0.2761 (1)	0.0873 (1)	0.045 (1)
C5′	0.8265 (2)	0.2258 (1)	0.0751 (1)	0.042 (1)
C6′	0.8988 (1)	0.1947 (1)	0.0055 (1)	0.045 (1)
N7′	0.8770 (2)	0.1451 (1)	0.0353 (1)	0.054 (1)
C8′	0.7965 (1)	0.1466 (1)	0.1184 (1)	0.053 (1)
N9′	0.7606 (1)	0.1949 (1)	0.1474 (1)	0.045 (1)
C10′	0.6706 (2)	0.2118 (1)	0.2304 (1)	0.044 (1)
C11′	0.5977 (1)	0.1785 (1)	0.2956 (1)	0.054 (1)
C12′	0.5081 (2)	0.1966 (1)	0.3742 (1)	0.060 (1)
C13′	0.4940 (2)	0.2475 (1)	0.3901 (1)	0.061 (1)
C14′	0.5666 (2)	0.2809 (1)	0.3253 (1)	0.055 (1)

C15′	0.6543 (2)	0.2632 (1)	0.2438 (1)	0.045 (1)
C16′	0.7274 (1)	0.2969 (1)	0.1706 (1)	0.044 (1)
N1A′	1.1155 (2)	0.1850 (1)	−0.2272 (1)	0.063 (1)
O2A′	1.0424 (1)	0.1655 (1)	−0.1370 (1)	0.059 (1)
C3A′	0.9830 (2)	0.2050 (1)	−0.0871 (1)	0.045 (1)
N4A′	1.0102 (2)	0.2471 (1)	−0.1341 (1)	0.051 (1)
C5A′	1.0915 (2)	0.2327 (1)	−0.2198 (1)	0.053 (1)
C1B′	1.1451 (2)	0.2688 (1)	−0.2970 (2)	0.065 (1)
C2B′	1.1857 (2)	0.3203 (1)	−0.2581 (1)	0.068 (1)
C3B′	1.0427 (2)	0.3126 (1)	−0.3249 (1)	0.066 (1)

Table 2. *Selected geometric parameters* (Å, °)

N1—C16	1.275 (2)	N1′—C16′	1.274 (2)
N1—C2	1.470 (2)	N1′—C2′	1.465 (2)
C2—C3	1.532 (2)	C2′—C3′	1.537 (2)
C3—N4	1.467 (1)	C3′—N4′	1.461 (1)
N4—C5	1.366 (1)	N4′—C5′	1.366 (1)
N4—C16	1.398 (1)	N4′—C16′	1.399 (1)
C5—N9	1.378 (1)	C5′—N9′	1.375 (1)
C5—C6	1.383 (2)	C5′—C6′	1.383 (2)
C6—N7	1.396 (1)	C6′—N7′	1.397 (1)
C6—C3A	1.435 (2)	C6′—C3A′	1.432 (2)
N7—C8	1.290 (2)	N7′—C8′	1.286 (2)
C8—N9	1.383 (2)	C8′—N9′	1.386 (2)
N9—C10	1.408 (1)	N9′—C10′	1.409 (2)
C10—C11	1.386 (2)	C10′—C11′	1.386 (2)
C10—C15	1.398 (2)	C10′—C15′	1.394 (2)
C11—C12	1.378 (2)	C11′—C12′	1.376 (2)
C12—C13	1.387 (2)	C12′—C13′	1.384 (2)
C13—C14	1.377 (2)	C13′—C14′	1.383 (2)
C14—C15	1.394 (2)	C14′—C15′	1.391 (2)
C15—C16	1.459 (2)	C15′—C16′	1.457 (2)
N1A—C5A	1.297 (2)	N1A′—C5A′	1.299 (2)
N1A—O2A	1.423 (1)	N1A′—O2A′	1.426 (2)
O2A—C3A	1.340 (1)	O2A′—C3A′	1.347 (1)
C3A—N4A	1.301 (2)	C3A′—N4A′	1.298 (2)
N4A—C5A	1.373 (2)	N4A′—C5A′	1.372 (2)
C5A—C1B	1.464 (2)	C5A′—C1B′	1.462 (2)
C1B—C2B	1.491 (2)	C1B′—C3B′	1.499 (2)
C1B—C3B	1.494 (2)	C1B′—C2B′	1.501 (2)
C2B—C3B	1.473 (2)	C2B′—C3B′	1.475 (2)
C16—N1—C2	106.9 (1)	C16′—N1′—C2′	107.0 (1)
N1—C2—C3	107.3 (1)	N1′—C2′—C3′	107.6 (1)
N4—C3—C2	100.9 (1)	N4′—C3′—C2′	101.1 (1)
C5—N4—C16	122.8 (1)	C5′—N4′—C16′	123.1 (1)
C5—N4—C3	127.4 (1)	C5′—N4′—C3′*	128.5 (1)
C16—N4—C3	108.1 (1)	C16′—N4′—C3′	108.3 (1)
N4—C5—N9	117.5 (1)	N4′—C5′—N9′	117.4 (1)
N4—C5—C6	136.5 (1)	N4′—C5′—C6′	136.7 (1)
N9—C5—C6	105.9 (1)	N9′—C5′—C6′	105.8 (1)
C5—C6—N7	109.2 (1)	C5′—C6′—N7′	109.4 (1)
C5—C6—C3A	131.9 (1)	C5′—C6′—C3A′	131.7 (1)
N7—C6—C3A	118.9 (1)	N7′—C6′—C3A′	119.0 (1)
C8—N7—C6	106.2 (1)	C8′—N7′—C6′	106.0 (1)
N7—C8—N9	112.3 (1)	N7′—C8′—N9′	112.4 (1)
C5—N9—C8	106.4 (1)	C5′—N9′—C8′	106.4 (1)
C5—N9—C10	124.1 (1)	C5′—N9′—C10′	124.1 (1)
C8—N9—C10	129.5 (1)	C8′—N9′—C10′	129.5 (1)
C11—C10—C15	120.6 (1)	C11′—C10′—C15′	120.8 (1)
C11—C10—N9	121.6 (1)	C11′—C10′—N9′	121.2 (1)
C15—C10—N9	117.9 (1)	C15′—C10′—N9′	118.2 (1)
C12—C11—C10	119.4 (1)	C12′—C11′—C10′	119.3 (1)
C11—C12—C13	120.4 (1)	C11′—C12′—C13′	120.6 (2)
C14—C13—C12	120.5 (1)	C14′—C13′—C12′	120.3 (1)
C13—C14—C15	119.8 (2)	C13′—C14′—C15′	119.8 (1)
C14—C15—C10	119.2 (1)	C14′—C15′—C10′	119.1 (1)
C14—C15—C16	121.8 (1)	C14′—C15′—C16′	121.7 (1)
C10—C15—C16	119.0 (1)	C10′—C15′—C16′	119.1 (1)
N1—C16—N4	115.5 (1)	N1′—C16′—N4′	115.8 (1)
N1—C16—C15	126.2 (1)	N1′—C16′—C15′	126.1 (1)
N4—C16—C15	118.3 (1)	N4′—C16′—C15′	118.2 (1)
C5A—N1A—O2A	103.1 (1)	C5A′—N1A′—O2A′	103.0 (1)
C3A—O2A—N1A	106.3 (1)	C3A′—O2A′—N1A′	106.1 (1)
N4A—C3A—O2A	112.8 (1)	N4A′—C3A′—O2A′	112.8 (1)
N4A—C3A—C6	131.2 (1)	N4A′—C3A′—C6′*	130.5 (1)
O2A—C3A—C6	115.9 (1)	O2A′—C3A′—C6′*	116.7 (1)
C3A—N4A—C5A	103.1 (1)	C3A′—N4A′—C5A′	103.1 (1)
N1A—C5A—N4A	114.7 (1)	N1A′—C5A′—N4A′	115.0 (1)
N1A—C5A—C1B	121.8 (1)	N1A′—C5A′—C1B′*	123.1 (1)
N4A—C5A—C1B	123.5 (1)	N4A′—C5A′—C1B′*	121.9 (1)
C5A—C1B—C2B	118.5 (1)	C5A′—C1B′—C3B′	118.1 (1)
C5A—C1B—C3B	119.7 (1)	C5A′—C1B′—C2B′*	117.7 (2)
C2B—C1B—C3B	59.1 (1)	C3B′—C1B′—C2B′	58.9 (1)
C3B—C2B—C1B	60.5 (1)	C3B′—C2B′—C1B′	60.6 (1)
C2B—C3B—C1B	60.3 (1)	C2B′—C3B′—C1B′	60.7 (1)
C5—C6—C3A—N4A	−4.7 (2)		
N7—C6—C3A—N4A	175.3 (1)		
C5—C6—C3A—O2A	174.2 (1)		
N7—C6—C3A—O2A	−5.8 (2)		
N1A—C5A—C1B—C2B	−149.3 (1)		
N4A—C5A—C1B—C2B	29.4 (2)		
N1A—C5A—C1B—C3B	141.9 (1)		
N4A—C5A—C1B—C3B	−39.4 (2)		
C5A—C1B—C2B—C3B	−109.4 (2)		
C5A—C1B—C3B—C2B	107.4 (1)		
C5′—C6′—C3A′—N4A′*	−2.8 (2)		
N7′—C6′—C3A′—N4A′	175.4 (1)		
C5′—C6′—C3A′—O2A′*	178.8 (1)		
N7′—C6′—C3A′—O2A′*	−3.0 (2)		
N1A′—C5A′—C1B′—C3B′	149.3 (2)		
N4A′—C5A′—C1B′—C3B′*	31.4 (3)		
N1A′—C5A′—C1B′—C2B′*	−143.1 (2)		
N4A′—C5A′—C1B′—C2B′*	−36.3 (2)		
C5A′—C1B′—C2B′—C3B′	−107.1 (2)		
C5A′—C1B′—C3B′—C2B′*	107.7 (2)		

* Denotes a parameter which differs significantly in value between molecules 1 and 2.

Table 3. *Least-squares-planes data*

Molecule 1, diimidazoquinazoline group

Equation of plane: 7.023 (1)x + 6.564 (7)y + 6.164 (2)z = 11.604 (3)

Deviation of atoms from the plane (Å):
(* Denotes an atom included in the calculation of the least-squares plane)

Diimidazoquinazoline group (rings *C*, *D*, *E* and *F*)			
C6*	0.044 (1)	C15*	−0.009 (1)
N7*	0.046 (1)	C14*	0.020 (1)
C8*	−0.008 (1)	C13*	0.041 (1)
N9*	−0.040 (1)	C12*	0.014 (1)
C5*	−0.010 (1)	C11*	−0.038 (1)
N4*	−0.045 (1)	C10*	−0.039 (1)
C16*	0.025 (1)		
N1	0.117 (2)	C2	0.084 (2)
C3	0.181 (2)		
Oxadiazole ring *A*			
N1A	0.295 (2)	N4A	0.022 (2)
O2A	0.259 (2)	C5A	0.148 (2)
C3A	0.093 (2)		
Cyclopropyl ring *B*			
C1B	0.144 (3)	C3B	−0.786 (3)
C2B	0.656 (3)		

R.m.s. deviation of fitted atoms from plane = 0.032 Å

Molecule 1, oxadiazole ring *A*

Equation of plane: 6.471 (4)x + 9.232 (16)y + 6.656 (7)z = 12.633 (6)

Deviation of atoms from the plane (Å):
(* Denotes an atom included in the calculation of the least-squares plane)

Oxadiazole ring *A*			
N1A*	0.001 (1)	N4A*	0.002 (1)
O2A*	0.000 (1)	C5A*	−0.002 (1)
C3A*	−0.001 (1)		
Cyclopropyl ring *B*			
C1B	0.017 (3)	C3B	−0.785 (3)
C2B	0.682 (3)		

R.m.s. deviation of fitted atoms from plane = 0.002 Å

Molecule 1, cyclopropyl ring *B*

Equation of plane: 5.477 (10)x − 3.285 (36)y + 10.022 (12)z = 6.077 (24)

Interplanar dihedral angles in molecule 1 (°)

Diimidazoquinazoline ring–oxadiazole ring	7.08 (7)
Diimidazoquinazoline ring–cyclopropyl ring	82.64 (7)
Oxadiazole ring–cyclopropyl ring	85.82 (7)

Molecule 2, diimidazoquinazoline group

Equation of plane: 6.833 (1)x + 0.446 (7)y + 7.203 (2)z = 6.311 (2)

Deviation of atoms from the plane (Å):
(* Denotes an atom included in the calculation of the least-squares plane)

Diimidazoquinazoline group (rings *C*′, *D*′, *E*′ and *F*′)

C6′*	−0.043 (1)	C15′*	0.033 (1)
N7′*	0.001 (1)	C14′*	0.029 (1)
C8′*	0.051 (1)	C13′*	−0.015 (1)
N9′*	0.036 (1)	C12′*	−0.056 (1)
C5′*	−0.021 (1)	C11′*	−0.018 (1)
N4′*	−0.044 (1)	C10′*	0.026 (1)
C16′*	0.021 (1)		
N1′	0.036 (2)	C2′	−0.045 (2)
C3′	−0.036 (2)		

Oxadiazole ring *A*′

N1*A*′	−0.242 (2)	N4*A*′	−0.263 (2)
O2*A*′	−0.101 (2)	C5*A*′	−0.332 (2)
C3*A*′	−0.130 (2)		

Cyclopropyl ring *B*′

C1*B*′	−0.506 (3)	C3*B*′	−1.386 (3)
C2*B*′	0.076 (3)		

R.m.s. deviation of fitted atoms from plane = 0.034 Å

Molecule 2, oxadiazole ring *A*′

Equation of plane: 7.175 (3)x + 2.605 (18)y + 6.404 (7)z = 7.031 (6)

Deviation of atoms from the plane (Å):
(* Denotes an atom included in the calculation of the least-squares plane)

Oxadiazole ring *A*′

N1*A*′*	0.000 (1)	N4*A*′*	0.002 (1)
O2*A*′*	0.002 (1)	C5*A*′*	−0.001 (1)
C3*A*′*	−0.002 (1)		

Cyclopropyl ring *B*′

C1*B*	−0.017 (3)	C3*B*	−0.816 (4)
C2*B*	0.658 (4)		

R.m.s. deviation of fitted atoms from plane = 0.002 Å

Molecule 2, cyclopropyl ring *B*′

Equation of plane: 4.745 (11)x − 4.318 (36)y + 10.659 (10)z = 9.760 (13)

Interplanar dihedral angles in molecule 2 (°)

Diimidazoquinazoline ring–oxadiazole ring	6.24 (7)
Diimidazoquinazoline ring–cyclopropyl ring	85.63 (6)
Oxadiazole ring–cyclopropyl ring	89.49 (7)

Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*92 (Sheldrick, 1992). Molecular graphics: *SNOOPI* (Davies, 1982).

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: LI1112). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Davies, E. K. (1982). *SNOOPI*. Chemical Crystallography Laboratory, Univ. of Oxford, England.

Im, H. K., Im, W. B., Pregenzer, F. F., Petke, J. D., Hamilton, B. J., Carter, D. B., von Voigtlander, P. F., Hansen, H. C. & Kristiansen, M. (1992). *Br. J. Pharmacol.* **107**, 622–627.

Sheldrick, G. M. (1985). *SHELXS86. Program for the Solution of Crystal Structures.* Univ. of Göttingen, Germany.

Sheldrick, G. M. (1992). *SHELXL92. Program for the Refinement of Crystal Structures.* Univ. of Göttingen, Germany.

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Polymorph (II) of Methyl 3-(4-Ethoxy-α-hydroxyiminobenzyl)-1,2,2-trimethylcyclopentanecarboxylate

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Abstract

The title compound, $C_{19}H_{27}NO_4$, is an intermediate product in the synthesis of oxazepinic and piperidinic compounds. Two crystalline forms of the title compound have been obtained but only one [form (II)] gave suitable crystals for X-ray structure analysis. The five-membered ring has an envelope conformation with C(2) 0.60 (5) Å out of the plane defined by the other four atoms. It has been established that the oxime group has a *syn* conformation and the two enantiomers form a dimer around the centre of symmetry by means of hydrogen bonds between their oxime groups.

Comment

The starting material for the synthesis of these oximes is camphoric anhydride (Chevallet *et al.*, 1988). Recrystallization of methyl 3-(4-ethoxy-α-hydroxyiminobenzyl)-1,2,2-trimethylcyclopentane-