$S = 1.101$
1833 reflections
204 parameters
H atoms located from difference Fourier map, refined isotropically

$(\Delta/\sigma)_{max} = -0.012$
$\Delta\rho_{max} = 0.217$ e Å^{-3}
$\Delta\rho_{min} = -0.275$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

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

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

	x	y	z	U_{eq}
N1	−0.1875 (2)	0.9383 (2)	0.3290 (2)	0.0286 (3)
C2	−0.1442 (3)	0.9126 (3)	0.1883 (2)	0.0342 (4)
C3	0.0334 (3)	0.7721 (3)	0.0990 (2)	0.0350 (5)
C4	0.1598 (3)	0.6584 (2)	0.1589 (2)	0.0295 (4)
C5	0.2275 (3)	0.5613 (2)	0.3849 (2)	0.0248 (4)
S5	0.46253 (6)	0.37538 (6)	0.28737 (5)	0.0300 (2)
O51	0.6031 (2)	0.4520 (2)	0.2071 (2)	0.0543 (4)
O52	0.4289 (2)	0.2778 (2)	0.1928 (2)	0.0388 (3)
O53	0.5119 (3)	0.2743 (2)	0.4018 (2)	0.0552 (5)
C6	0.1631 (3)	0.5931 (2)	0.5323 (2)	0.0267 (4)
C7	−0.0141 (3)	0.7450 (2)	0.6128 (2)	0.0264 (4)
N7	−0.0714 (2)	0.7654 (2)	0.7703 (2)	0.0308 (4)
O71	−0.1633 (3)	0.9180 (2)	0.8341 (2)	0.0490 (4)
O72	−0.0238 (2)	0.6305 (2)	0.83082 (15)	0.0396 (3)
C8	−0.1325 (3)	0.8675 (2)	0.5494 (2)	0.0262 (4)
O8	−0.3001 (2)	1.0156 (2)	0.6092 (2)	0.0373 (3)
C9	−0.0676 (3)	0.8271 (2)	0.3953 (2)	0.0243 (4)
C10	0.1107 (2)	0.6789 (2)	0.3108 (2)	0.0241 (4)
O′	−0.5392 (3)	1.1988 (3)	0.8649 (2)	0.0617 (5)

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

N1—C2	1.317 (3)	S5—O53	1.451 (2)
N1—C9	1.368 (2)	C7—N7	1.455 (2)
C5—S5	1.786 (2)	N7—O72	1.221 (2)
S5—O51	1.443 (2)	N7—O71	1.231 (2)
S5—O52	1.444 (1)	C8—O8	1.323 (2)
C2—N1—C9	122.8 (2)	O53—S5—C5	104.10 (9)
C6—C5—S5	118.6 (1)	C8—C7—N7	120.5 (2)
C10—C5—S5	121.5 (1)	C6—C7—N7	116.4 (2)
O51—S5—O52	112.8 (1)	O72—N7—O71	124.0 (2)
O51—S5—O53	113.1 (1)	O72—N7—C7	118.1 (2)
O52—S5—O53	112.96 (9)	O71—N7—C7	117.9 (2)
O51—S5—C5	105.26 (9)	O8—C8—C7	130.1 (2)
O52—S5—C5	107.72 (8)	O8—C8—C9	114.6 (2)

Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: VJ1030). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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A Non-Peptide Angiotensin II Receptor Antagonist: 2-Butyl-6-dimethoxymethyl-5-phenyl-1-{[2′-(1*H*-tetrazol-5-yl)biphenyl-4-yl]methyl}-1*H*-imidazo[5,4-*b*]pyridine

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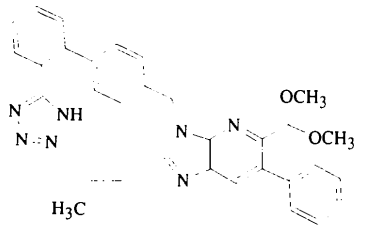
Abstract

The title compound, $C_{33}H_{33}N_7O_2$, is one of a series of imidazo[4,5-*b*]pyridine-based angiotensin II receptor antagonists showing high antihypertensive activity. The biphenyltetrazole moiety assumes the same conformation as in related compounds, but its relative orientation with respect to the central fused ring is different to that in these compounds, indicating that there is considerable conformational flexibility about the methylene bridge joining the two ring systems.

Comment

Non-peptide angiotensin II (AII) receptor antagonists such as losartan are being actively investigated for treatment of hypertension in humans (Duncia *et al.*, 1992). Most of them contain a biphenyltetrazole moiety linked to a heterocycle by a methylene group. The title

compound, (I), is an imidazo[4,5-*b*]pyridine-based AII antagonist with high antihypertensive activity. The X-ray analysis of this compound has been performed in order to establish its conformational characteristics.



(I)

An *ORTEP*II drawing (Johnson, 1976) of the molecule with the atomic numbering scheme is presented in Fig. 1. Molecular dimensions are normal within experimental error. The imidazopyridine ring is planar with a maximum deviation of 0.064 (10) Å for atom C5. The three phenyl rings and the tetrazole ring are also planar, with maximum deviations of 0.017 (9), 0.025 (12), 0.034 (15) and 0.027 (10) Å for atoms C16, C20, C35 and N24, respectively. The dihedral angle between the imidazopyridine and the C5-phenyl rings is 52.7 (5)°. The dihedral angles between the two phenyl rings and between the phenyl and tetrazole rings in the biphenyltetrazole moiety are 45.8 (5) and 58.8 (5)°, respectively. There is one intermolecular N27—H···N3 hydrogen bond [N···N($\frac{3}{2}-x$, $-\frac{1}{2}+y$, z) 2.802 (16), H···N 1.947 Å, N—H···N 172.5 (5)°]. There are no unusually close contacts shorter than van der Waals distances.

The crystal structure can be compared with that of 2-butyl-1-{[2′-(1*H*-tetrazol-5-yl)biphenyl-4-yl]methyl}-1*H*-benzimidazole-7-carboxylic acid reported by the Takeda group (Kubo *et al.*, 1993). Superimposed structures shown in Fig. 2 indicate that the overall conformations are similar in terms of the relative orientation of the biphenyltetrazole moiety with respect to the central heterocyclic ring. They also show that there is conformational flexibility about the bonds in the methylene bridge linking the two ring systems. Differences in the conformations are manifested in the C8—N1—C10—C11 and N1—C10—C11—C12 torsion angles listed in Table 3. The *n*-butyl side chain also assumes different conformations in the two compounds.

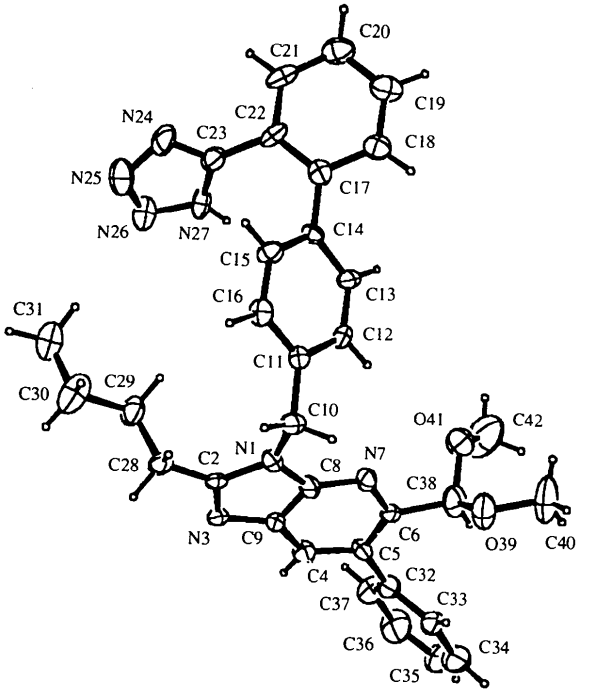


Fig. 1. *ORTEP*II view (Johnson, 1976) of the title compound, with the atomic numbering scheme and displacement ellipsoids drawn at the 25% probability level.

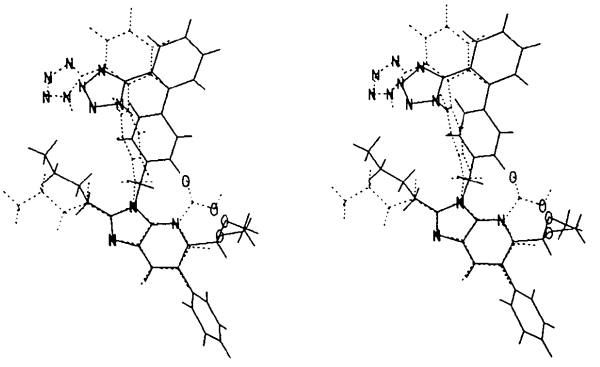


Fig. 2. Stereoscopic view of the superimposed structures of the title compound (solid line) and the Takeda (Kubo *et al.*, 1993) compound (dotted line).

From molecular-mechanics calculations, Bradbury *et al.* (1992, 1993) proposed that the biphenyltetrazole moiety can assume two enantiomeric minimum-energy conformations, with the planes of the phenyl rings twisted by ±61° and a barrier to planarity of 6.7 kcal mol^{-1}. In the crystal, the biphenyltetrazole moiety itself assumes the same conformation, as shown by the similar C13—C14—C17—C22 and C17—C22—C23—N27 torsion angles (Table 3). However, the twist angle between the phenyl rings is *ca* 45° rather than the 61° suggested by energy calculation. It is interesting to note that in all related crystal structures, the tetrazole rings are oriented in such a way that the protonated N27 atom is situated close to the phenyl ring, with a dihedral angle of *ca* 58°.

Experimental

The synthesis and biological evaluation of the title compound were carried out at the Korea Research Institute of Chemical Technology (unpublished results). Crystals were obtained from an ethanol solution. The density D_m was measured by flotation in an *n*-hexane/carbon tetrachloride solution.

Crystal data

$C_{33}H_{33}N_7O_2$
M_r = 559.66
Orthorhombic
Pbca
a = 20.738 (7) Å
b = 9.791 (3) Å
c = 30.251 (10) Å
V = 6142.4 (33) Å^3
Z = 8
D_x = 1.210 Mg m^{-3}
D_m = 1.20 Mg m^{-3}

Cu $K\alpha$ radiation
λ = 1.5418 Å
Cell parameters from 29 reflections
θ = 9.6–12.1°
μ = 0.626 mm^{-1}
T = 291 (2) K
Approximately round-shaped without any well developed faces
0.50 × 0.30 × 0.20 mm
Colorless

Data collection

Rigaku AFC-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
3678 measured reflections
3220 independent reflections
1220 observed reflections [$I > 2\sigma(I)$]

θ_{max} = 50.53°
$h = 0 \rightarrow 20$
$k = 0 \rightarrow 9$
$l = 0 \rightarrow 30$
2 standard reflections monitored every 50 reflections
intensity decay: 2%

Refinement

Refinement on F^2
$R(F)$ = 0.1066
$wR(F^2)$ = 0.3363
S = 1.327
3220 reflections
382 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.337
$\Delta\rho_{max}$ = 0.283 e Å^{-3}
$\Delta\rho_{min}$ = −0.324 e Å^{-3}
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

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

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

	x	y	z	U_{eq}
N1	0.7344 (5)	0.0498 (11)	0.6032 (4)	0.068 (3)
C2	0.7056 (7)	0.0772 (14)	0.5629 (5)	0.063 (4)
N3	0.6453 (5)	0.0269 (12)	0.5612 (3)	0.069 (3)
C4	0.5811 (6)	−0.0953 (13)	0.6222 (5)	0.067 (4)
C5	0.5847 (7)	−0.1331 (13)	0.6662 (4)	0.061 (4)
C6	0.6429 (7)	−0.1171 (14)	0.6872 (4)	0.061 (4)
N7	0.6969 (5)	−0.0638 (10)	0.6691 (4)	0.062 (3)
C8	0.6888 (7)	−0.0217 (15)	0.6282 (5)	0.071 (4)
C9	0.6322 (7)	−0.0354 (15)	0.6024 (4)	0.064 (4)
C10	0.7958 (6)	0.0949 (15)	0.6199 (4)	0.075 (4)
C11	0.8503 (6)	−0.0070 (14)	0.6159 (4)	0.058 (4)
C12	0.8520 (7)	−0.1313 (16)	0.6401 (4)	0.070 (4)
C13	0.9006 (6)	−0.2231 (15)	0.6371 (4)	0.065 (4)
C14	0.9543 (6)	−0.1970 (13)	0.6093 (4)	0.054 (3)
C15	0.9520 (7)	−0.0766 (14)	0.5860 (4)	0.070 (4)
C16	0.9027 (7)	0.0160 (14)	0.5874 (4)	0.068 (4)
C17	1.0089 (6)	−0.2883 (14)	0.6065 (5)	0.066 (4)
C18	1.0355 (7)	−0.3415 (16)	0.6454 (5)	0.081 (5)
C19	1.0871 (9)	−0.4317 (18)	0.6443 (6)	0.105 (6)
C20	1.1168 (9)	−0.4674 (17)	0.6042 (7)	0.107 (6)
C21	1.0890 (7)	−0.4175 (18)	0.5656 (6)	0.089 (5)
C22	1.0366 (8)	−0.3304 (15)	0.5671 (5)	0.075 (5)
C23	1.0072 (8)	−0.2920 (18)	0.5241 (5)	0.078 (5)
N24	1.0337 (7)	−0.2333 (14)	0.4904 (6)	0.098 (5)
N25	0.9868 (10)	−0.2193 (14)	0.4593 (4)	0.108 (5)
N26	0.9338 (7)	−0.2800 (15)	0.4723 (5)	0.103 (5)
N27	0.9464 (7)	−0.3240 (11)	0.5133 (4)	0.081 (4)
C28	0.7364 (8)	0.1451 (15)	0.5254 (4)	0.091 (5)
C29	0.7700 (7)	0.0495 (17)	0.4948 (4)	0.095 (5)
C30	0.8018 (10)	0.1274 (21)	0.4569 (6)	0.149 (8)
C31	0.8351 (9)	0.0269 (24)	0.4278 (6)	0.180 (10)
C32	0.5254 (8)	−0.1824 (18)	0.6875 (5)	0.081 (5)
C33	0.5034 (9)	−0.1229 (16)	0.7271 (5)	0.085 (5)
C34	0.4477 (10)	−0.1594 (21)	0.7477 (7)	0.113 (6)
C35	0.4107 (10)	−0.2639 (25)	0.7297 (8)	0.133 (9)
C36	0.4297 (10)	−0.3165 (22)	0.6898 (7)	0.144 (8)
C37	0.4878 (9)	−0.2787 (18)	0.6698 (6)	0.107 (6)
C38	0.6538 (10)	−0.1801 (18)	0.7334 (5)	0.100 (6)
O39	0.6760 (6)	−0.0762 (12)	0.7598 (4)	0.124 (4)
C40	0.6905 (11)	−0.1196 (25)	0.8045 (5)	0.220 (12)
O41	0.7056 (6)	−0.2737 (14)	0.7301 (4)	0.115 (4)
C42	0.6860 (13)	−0.3952 (25)	0.7440 (8)	0.232 (14)

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

N1—C2	1.382 (14)	C14—C17	1.44 (2)
N1—C8	1.40 (2)	C22—C23	1.48 (2)
N1—C10	1.441 (14)	C23—N24	1.29 (2)
C2—N3	1.34 (2)	C23—N27	1.34 (2)
C2—C28	1.46 (2)	N24—N25	1.36 (2)
N3—C9	1.414 (15)	N25—N26	1.31 (2)
C4—C9	1.35 (2)	N26—N27	1.339 (14)
C4—C5	1.38 (2)	C28—C29	1.49 (2)
C5—C6	1.37 (2)	C29—C30	1.53 (2)
C6—N7	1.351 (15)	C30—C31	1.49 (2)
C6—C38	1.54 (2)	C38—O39	1.37 (2)
N7—C8	1.315 (14)	C38—O41	1.42 (2)
C8—C9	1.41 (2)	O39—C40	1.45 (2)
C10—C11	1.51 (2)	O41—C42	1.32 (2)
C2—N1—C8	106.3 (11)	C18—C17—C14	119.3 (14)
C2—N1—C10	129.2 (13)	C21—C22—C17	122.6 (16)
C8—N1—C10	124.2 (12)	C21—C22—C23	116.8 (15)
N3—C2—N1	111.4 (12)	C17—C22—C23	120.5 (15)
N3—C2—C28	122.8 (14)	N24—C23—N27	108.1 (14)
N1—C2—C28	125.7 (14)	N24—C23—C22	128.9 (17)
C2—N3—C9	107.6 (11)	N27—C23—C22	122.8 (16)
C9—C4—C5	120.0 (13)	C23—N24—N25	106.7 (13)
C6—C5—C4	117.6 (13)	N26—N25—N24	110.2 (13)
N7—C6—C5	125.7 (12)	N25—N26—N27	105.1 (13)
N7—C6—C38	113.6 (13)	C23—N27—N26	109.6 (13)
C5—C6—C38	120.1 (14)	C2—C28—C29	113.6 (12)
C8—N7—C6	113.4 (12)	C28—C29—C30	110.8 (14)
N7—C8—N1	125.4 (14)	C31—C30—C29	108.3 (17)
N7—C8—C9	126.5 (14)	C37—C32—C5	122.9 (17)
N1—C8—C9	108.1 (12)	O39—C38—O41	105.5 (15)
C4—C9—C8	116.6 (13)	O39—C38—C6	106.2 (13)
C4—C9—N3	136.7 (14)	O41—C38—C6	107.8 (13)
C8—C9—N3	106.6 (13)	C38—O39—C40	113.3 (14)
N1—C10—C11	115.5 (12)	C42—O41—C38	109.1 (17)
C22—C17—C14	124.0 (14)		
C2—N1—C10—C11	−98.8 (16)	C28—C29—C30—C31	179.5 (15)
N1—C10—C11—C12	−67.4 (17)	C4—C5—C32—C33	−126.5 (15)
C13—C14—C17—C18	−45.0 (18)	C5—C6—C38—O39	−127.7 (15)
C17—C22—C23—N24	127.0 (17)	C5—C6—C38—O41	119.6 (15)
N1—C2—C28—C29	89.1 (18)	C6—C38—O39—C40	−178.3 (14)
C2—C28—C29—C30	−179.2 (14)	C6—C38—O41—C42	−123.7 (17)

Table 3. *Comparison of torsion angles (°) involving the biphenyltetrazole moiety in the title and related compounds*

φ_1 = C8—N1—C10—C11, φ_2 = N1—C10—C11—C12, φ_3 = C13—C14—C17—C22 and φ_4 = C17—C22—C23—N27.

	φ_1	φ_2	φ_3	φ_4
(I)	∓88.3 (15)	±67.4 (17)	∓133.5 (14)	±57.8 (21)
(II)	∓105.2 (7)	±32.1 (6)	∓135.7 (8)	±54.5 (7)
(III)	∓111.6	±71.2	∓143.7	±57.6
(IV)			∓139.6	±57.0

Notes: (I) this compound; (II) Takeda compound (Kubo *et al.*, 1993); (III) 5,8-dihydro-2,4-dimethyl-8-{[2′-(1*H*-tetrazol-5-yl)biphenyl-4-yl]-methyl}pyrido[2,3-*d*]pyrimidin-7(6*H*)-one (Ellingboe *et al.*, 1994); (IV) 2-ethyl-5,6,7,8-tetrahydro-4-{[2′-(1*H*-tetrazol-5-yl)biphenyl-4-yl]methoxyl}quinolone (Bradbury *et al.*, 1993); all the crystal structures are in centrosymmetric space groups.

X-ray data were collected using standard techniques. Diffraction from the crystals was generally very weak and only 38% of the reflections were observed with $I > 2\sigma(I)$. Crystals of better quality were not available. H atoms were generated geometrically and refined using the *AFIX* option of *SHELXL*93 (Sheldrick, 1993), except for the methyl H atoms which were found from a difference Fourier map and refined using the *AFIX* 137 option. The isotropic displacement parameters of all H atoms were fixed as 1.2 times the isotropic equivalents of their bonded atoms.

Data collection: local program (Yoon, Kim & Shin, 1994). Cell refinement: local program. Data reduction: local program. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*93. Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *SHELXL*93.

This work was supported by the Ministry of Science and Technology, Korea.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: KH1056). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Ipriflavone, an Antiostheophorotic Agent

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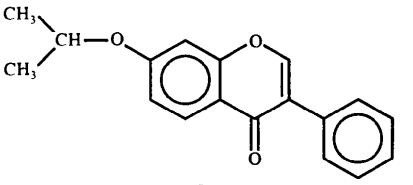
Abstract

The antiostheophorotic agent ipriflavone [7-(1-methylethoxy)-3-phenyl-4*H*-1-benzopyran-4-one, $C_{18}H_{16}O_3$] is an important member of the isoflavone family. The structure of the molecule is dominated by the dihedral angle (50°) between the planes of the phenyl and benzopyran moieties. A structural comparison with other related published structures is represented.

Comment

Isoflavone derivatives are widely known to be biologically active compounds. A number of publications report crystal structures of isoflavone derivatives (Shoja, 1992*a*,*b*; Acharya, Puranik, Tavale & Guru Row, 1986; Breton, Precigoux, Courseille & Hospital, 1975) including naturally occurring molecules. Licoricone (Kaneda, Iitaka & Shibata, 1973) from the root of licorice, for example, is used in the treatment of stomach ulcers. Aformosine (Caballero & Smith, 1986) is an isoflavone partly responsible for the insect resistance of a soybean species.

Ipriflavone, (I) (Feuer, Nógrádi, Gottsegen, Vermes, Streliszky, Wolfner, Farkas, Antus, Kovács, 1971; Lányi, Nógrádi, Ecsery-Puskás & Hermecz, 1995; Varga, Bátori, Hermecz, 1995), has been registered 19 years after its synthesis and launched as an effective ostheophorotic agent, first in Japan in 1988 (registered names: Osteochin in Hungary, Osten in Japan, Osteofix in Italy). A crystal structure analysis of (I) has been carried out in order to contribute to a wider structural characterization of the active substance of the drug.



(I)

The molecule consists of a planar phenyl ring and a planar 7-isopropoxy-substituted benzopyran moiety. The two planar moieties form an angle of 50.0°. Considering