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Platelet Activating Factor Antagonist Design. 3. X-ray Crystal Structure and Intermolecular Crystal Lattice Interactions of Methyl *trans*-4-Acetoxymethyl-4,5-dihydro-2,5-bis(3,4-methylenedioxyphenyl)-3-furancarboxylate

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Abstract. $C_{23}H_{20}O_9$, $M_r = 440{\cdot}41$, monoclinic, $P2_1/c$, $a = 11{\cdot}433$ (1), $b = 7{\cdot}808$ (2), $c = 23{\cdot}313$ (3) Å, $\beta = 99{\cdot}67$ (1)°, $V = 2052$ Å^3, $Z = 4$, $D_x = 1{\cdot}43$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 0{\cdot}69$ cm^{-1}, $F(000) = 920$, $T = 293$ K, final $R = 0{\cdot}048$ for 1645 observed [$F_o \geq 5\sigma(F_o)$] reflections. The observed structure reveals a *trans* relationship for the 4-acetoxymethyl and 5-aryl substituents. The 4,5-dihydrofuran ring system adopts an envelope conformation. There is no crystallographically imposed symmetry. Several intermolecular van der Waals interactions occur in the cell lattice of this compound.

Introduction. Platelet-activating-factor (PAF) is an important mediator of mammalian cell function and it is thought to play a significant role in several alterations of the pulmonary, intravascular, and cardiovascular systems (Venuti, 1985; McManus, 1986; Etienne, Hecquet & Braquet, 1988; Smith, Rubin & Patterson, 1988). The specific binding of PAF to cellular membrane receptor sites is the first step in its biological functions (McManus, 1986; Hwang, Lam, Biftu, Beattie & Shen, 1985). Potent and selective PAF antagonists provide leads to the molecular characteristics of the PAF receptor site in addition to serving as therapeutically effective agents (Braquet & Godfroid, 1986; Godfroid & Braquet, 1986; Corey, Chen & Parry, 1988). We recently reported some early investigations aimed at the design of such antagonists (Peterson, Smillie & Rogers, 1989; Peterson, Do & Rogers, 1989), which were modeled upon naturally occurring furanoid lignans (Braquet & Godfroid, 1986; Biftu & Stevenson, 1987) and Merck Sharp & Dohme's potent PAF antagonists L-652,732 and L-659,989 (Hwang *et al.*, 1985; Biftu, Gamble, Doebber, Hwang, Shen, Snyder, Springer & Stevenson, 1986; Wu, Biftu & Doebber, 1986; Ponpipom, Hwang, Doebber, Acton, Alberts, Biftu, Brooker, Bugianesi, Chabala, Gamble, Graham, Lam & Wu, 1988). In our approach, X-ray crystallography is projected to provide not only detail about the three-dimensional topography of a compound and its congeneric series, but also information about the molecular nature of the biological receptor site through an understanding of the intermolecular interactions that stabilize the crystal lattice (Codding & Muir, 1985; Codding, 1988). Herein we describe the X-ray crystal structure and an analysis of the closest contacts between neighboring molecules in the crystal lattice for the title compound, prepared en route to hinokin, a phytolignan member of the PAF-antagonistic family of prestegane natural products (Braquet & Godfroid, 1986).

Experimental. The title dihydrofuran was prepared in 43% isolated yield by manganese(III) acetate oxidation

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of methyl 3,4-methylenedioxybenzoylacetate in the presence of *trans*-3-(3,4-methylenedioxyphenyl)-2-propen-1-ol acetate (Yang, Trost & Fristad, 1987). The product was purified by flash chromatography on silica gel while eluting with 15% ethyl acetate in petroleum ether. Crystals (m.p. 373–374 K) were obtained by slow evaporation of a methanol solution of the title compound. The X-ray structure was in full agreement with the spectral and analytical data.* D_m not determined. Crystal 0·15 × 0·20 × 0·25 mm. Enraf–Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$. Cell constants from setting angles of 25 reflections ($\theta > 19°$). Correction for Lorentz–polarization effect. $\theta_{max} = 50°$; h 0 to 13, k 0 to 9, l −27 to 27. Standard reflections observed every 3600 s of data-collection time (500, 020, 006), variation = ±2%. 4080 reflections measured, 1645 independent observed reflections [$F_o \geq 5\sigma(F_o)$]. Structure solved utilizing *MULTAN* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) direct-methods program. Least-squares refinement with isotropic thermal parameters led to $R = 0·108$. The geometrically constrained H atoms were placed in calculated positions 0·95 Å from the bonded C atom and allowed to ride on that atom with B fixed at 5·5 Å^2. The methyl H atoms were included as a rigid group with rotational freedom at the bonded C atom (C—H = 0·95 Å, B = 5·5 Å^2). Scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974); structure refined with *SHELX76* (Sheldrick, 1976). $\sum w(|F_o| - |F_c|)^2$ minimized, weights = $[\sigma(F_o)^2 + 0·0001F_o^2]^{-1}$, 295 parameters varied. $R = 0·048$, $wR = 0·048$, $S = 0·80$. Δ/σ in final least-squares refinement cycle <0·01, $\Delta\rho < 0·2$ e Å^{-3} in final difference map.

Discussion. Fractional coordinates and B_{eq} values are given in Table 1,† bond distances and angles in Table 2, and an *ORTEP* drawing (Johnson, 1976) in Fig. 1. A cell plot is provided in Fig. 2.

The observed structure reveals a *trans* stereochemical disposition for the substituents about C(3) and C(4). Consistent with this finding is the C(21)–C(3)–C(4)–C(5) torsion angle of 140·3° and the

Table 1. *Final fractional coordinates and equivalent isotropic thermal parameters*

	x	y	z	B_{eq}* (Å^2)
O(1)	0·2844 (2)	0·0351 (4)	0·1632 (1)	2·28
O(2)	0·7571 (3)	−0·3062 (5)	0·1439 (1)	2·82
O(3)	0·6887 (3)	−0·3064 (5)	0·0446 (1)	3·49
O(4)	−0·0023 (3)	0·2882 (4)	−0·0067 (1)	2·91
O(5)	−0·1912 (3)	0·2458 (5)	0·0145 (1)	3·07
O(6)	0·0382 (3)	−0·3865 (5)	0·1506 (2)	4·01
O(7)	0·1738 (3)	−0·4869 (4)	0·2220 (1)	3·06
O(8)	0·4539 (3)	−0·1597 (5)	0·3132 (1)	2·87
O(9)	0·4001 (3)	−0·1999 (6)	0·4000 (1)	4·41
C(1)	0·1872 (4)	−0·0688 (6)	0·1574 (2)	2·00
C(2)	0·2080 (4)	−0·2169 (6)	0·1870 (2)	2·04
C(3)	0·3321 (4)	−0·2138 (6)	0·2212 (2)	2·02
C(4)	0·3859 (4)	−0·0626 (6)	0·1925 (2)	2·11
C(5)	0·4631 (4)	−0·1199 (6)	0·1486 (2)	2·13
C(6)	0·5771 (4)	−0·1808 (6)	0·1714 (2)	2·13
C(7)	0·6432 (4)	−0·2414 (6)	0·1324 (2)	2·07
C(8)	0·7794 (4)	−0·3713 (8)	0·0890 (2)	3·18
C(9)	0·6018 (4)	−0·2422 (7)	0·0732 (2)	2·44
C(10)	0·4922 (4)	−0·1854 (7)	0·0501 (2)	2·81
C(11)	0·4219 (4)	−0·1210 (6)	0·0894 (2)	2·45
C(12)	0·0832 (4)	0·0079 (6)	0·1205 (2)	1·97
C(13)	0·1013 (4)	0·1124 (6)	0·0737 (2)	2·14
C(14)	0·0025 (4)	0·1844 (6)	0·0415 (2)	2·03
C(15)	−0·1242 (4)	0·3355 (7)	−0·0221 (2)	2·81
C(16)	−0·1094 (4)	0·1612 (6)	0·0545 (2)	2·27
C(17)	−0·1296 (4)	0·0610 (7)	0·0998 (2)	2·67
C(18)	−0·0307 (4)	−0·0159 (6)	0·1328 (2)	2·46
C(19)	0·1295 (4)	−0·3662 (6)	0·1836 (2)	2·34
C(20)	0·1053 (5)	−0·6426 (7)	0·2191 (2)	3·75
C(21)	0·3314 (4)	−0·1863 (7)	0·2861 (2)	2·86
C(22)	0·4751 (5)	−0·1643 (7)	0·3725 (2)	2·82
C(23)	0·6008 (4)	−0·1158 (8)	0·3944 (2)	3·52

* $B_{eq} = \frac{4}{3}[a^2b_{11} + b^2b_{22} + c^2b_{33} + ab(\cos\gamma)b_{12} + ac(\cos\beta)b_{13} + bc(\cos\alpha)b_{23}]$.

Table 2. *Bond distances* (Å) *and angles* (°)

O(1)–C(1)	1·364 (5)	O(1)–C(4)	1·460 (5)
O(2)–C(7)	1·381 (5)	O(2)–C(8)	1·439 (5)
O(3)–C(8)	1·429 (5)	O(3)–C(9)	1·381 (5)
O(4)–C(14)	1·379 (5)	O(4)–C(15)	1·428 (5)
O(5)–C(15)	1·423 (5)	O(5)–C(16)	1·374 (5)
O(6)–C(19)	1·199 (5)	O(7)–C(19)	1·340 (5)
O(7)–C(20)	1·441 (6)	O(8)–C(21)	1·451 (5)
O(8)–C(22)	1·363 (5)	O(9)–C(22)	1·186 (6)
C(1)–C(2)	1·347 (6)	C(1)–C(12)	1·472 (6)
C(2)–C(3)	1·507 (5)	C(2)–C(19)	1·465 (6)
C(3)–C(4)	1·536 (6)	C(3)–C(21)	1·529 (6)
C(4)–C(5)	1·525 (6)	C(5)–C(6)	1·406 (6)
C(5)–C(11)	1·382 (5)	C(6)–C(7)	1·360 (6)
C(7)–C(9)	1·380 (6)	C(9)–C(10)	1·353 (6)
C(10)–C(11)	1·408 (6)	C(12)–C(13)	1·406 (6)
C(12)–C(18)	1·392 (5)	C(13)–C(14)	1·367 (6)
C(14)–C(16)	1·375 (6)	C(16)–C(17)	1·365 (6)
C(17)–C(18)	1·392 (6)	C(22)–C(23)	1·492 (7)

C(1)–O(1)–C(4)	107·8 (3)	C(7)–O(2)–C(8)	104·9 (3)
C(8)–O(3)–C(9)	105·8 (3)	C(14)–O(4)–C(15)	105·1 (4)
C(15)–O(5)–C(16)	105·6 (3)	C(19)–O(7)–C(20)	114·8 (4)
C(21)–O(8)–C(22)	115·6 (4)	O(1)–C(1)–C(2)	112·9 (4)
O(1)–C(1)–C(12)	112·4 (4)	C(2)–C(1)–C(12)	134·8 (4)
C(1)–C(2)–C(3)	109·1 (4)	C(1)–C(2)–C(19)	127·0 (4)
C(3)–C(2)–C(19)	123·7 (4)	C(2)–C(3)–C(4)	101·1 (3)
C(2)–C(3)–C(21)	111·4 (4)	C(4)–C(3)–C(21)	113·1 (4)
O(1)–C(4)–C(3)	105·1 (3)	O(1)–C(4)–C(5)	110·2 (3)
C(3)–C(4)–C(5)	112·7 (4)	C(4)–C(5)–C(6)	116·8 (4)
C(4)–C(5)–C(11)	122·2 (4)	C(6)–C(5)–C(11)	120·9 (4)
C(5)–C(6)–C(7)	116·7 (4)	O(2)–C(7)–C(6)	127·5 (4)
O(2)–C(7)–C(9)	110·3 (4)	C(6)–C(7)–C(9)	122·2 (4)
O(2)–C(8)–O(3)	107·7 (4)	O(3)–C(9)–C(7)	109·3 (4)
O(3)–C(9)–C(10)	128·3 (4)	C(7)–C(9)–C(10)	122·4 (5)
C(9)–C(10)–C(11)	116·7 (4)	C(5)–C(11)–C(10)	121·0 (4)
C(1)–C(12)–C(13)	118·7 (4)	C(1)–C(12)–C(18)	121·1 (4)
C(13)–C(12)–C(18)	120·1 (4)	C(12)–C(13)–C(14)	116·7 (4)
O(4)–C(14)–C(13)	127·2 (4)	O(4)–C(14)–C(16)	110·2 (4)
C(13)–C(14)–C(16)	122·6 (4)	O(4)–C(15)–O(5)	108·8 (4)
O(5)–C(16)–C(14)	109·9 (4)	O(5)–C(16)–C(17)	128·1 (4)
C(14)–C(16)–C(17)	122·0 (4)	C(16)–C(17)–C(18)	116·6 (4)
C(12)–C(18)–C(17)	122·0 (4)	O(6)–C(19)–O(7)	121·8 (5)
O(6)–C(19)–C(2)	126·8 (5)	O(7)–C(19)–C(2)	111·4 (4)
O(8)–C(21)–C(3)	106·6 (3)	O(8)–C(22)–O(9)	122·2 (5)
O(8)–C(22)–C(23)	109·7 (5)	O(9)–C(22)–C(23)	128·1 (5)

* Physical data: IR (KBr) 2905, 2840, 2790, 1730, 1690, 1595, 1480, 1440, 1370, 1360, 1315, 1230, 1155, 1100, 1070, 1035, 930, 860, 810, 750 cm^{-1}; ^{1}H NMR ($CDCl_3$, 200 MHz) δ 7·50 (*dd*, J = 8·28, 1·57 Hz, 1 H), 7·40 (*d*, J = 1·57 Hz, 1 H), 7·95–7·80 (*m*, 4 H), 6·02 (*s*, 2 H), 5·98 (*s*, 2 H), 5·41 (*d*, J = 4·42 Hz, 1 H), 4·43 (*dd*, J = 10·85, 3·65 Hz, 1 H), 4·29 (*dd*, J = 10·85, 7·95 Hz, 1 H), 3·68 (*s*, 3 H), 3·7–3·5 (*m*, 1 H), 2·10 (*s*, 3 H); analysis calculated for $C_{23}H_{20}O_9$: C, 62·70, H, 4·52%; found C, 62·63, H, 4·62%.

† Lists of structure factors, anisotropic thermal parameters, least-squares-planes results, torsion angles, and final fractional coordinates for H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51696 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

H(1)C(3)–C(3)–C(4)–H(1)C(4) torsion angle of −94·9°. The observed 4·42 Hz vicinal hydrogen coupling constant between C(4)–H and C(3)–H suggests some relaxation of these torsion angles when the compound is in solution (Karplus, 1963). Similar coupling constants ($J = 5$ Hz) have been reported for some related 3,4-disubstituted-2,5-diaryltetrahydrofurans (Cooper, Gottlieb, Lavie & Levy, 1979).

The dihydrofuran ring exists in an envelope conformation with ring atoms O(1), C(1), C(2) and C(3) describing a plane to within 0·022 Å. Ring atom C(4) deviates from this plane by 0·309 Å. The atoms C(1), C(2), O(1) and C(12) are planar to within 0·003 Å, and ring atoms C(3) and C(4) lie −0·114 and 0·216 Å out this plane, respectively. The C(1)–C(2)–O(1)–C(12) plane intersects the dihydrofuran ring plane at an angle of 3·26°. Similarly, atoms C(1), C(2), C(3) and C(19) define a plane that intersects the dihydrofuran ring plane at an angle of 5·18°. These atoms are within 0·028 Å of planarity. Ring atom O(1) deviates from the C(1)–C(2)–C(3)–C(19) plane by 0·161 Å and atom C(4) by 0·456 Å. As expected, the 2-aryl ring atoms C(12) through C(18) are planar to within 0·008 Å. This plane intersects the O(1)–C(1)–C(2)–C(3) plane at an angle of 35·89°. Methylenedioxy atoms O(4), O(5) and C(15) lie out of the 2-aryl ring plane by 0·028, 0·038 and −0·030 Å, respectively. Likewise, the 5-aryl ring atoms C(5) through C(7) and C(9) through C(11) describe a plane to within 0·006 Å. Methylenedioxy atom O(2) deviates from this plane by 0·010 Å, O(3) by 0·036 Å, and C(8) by −0·169 Å.

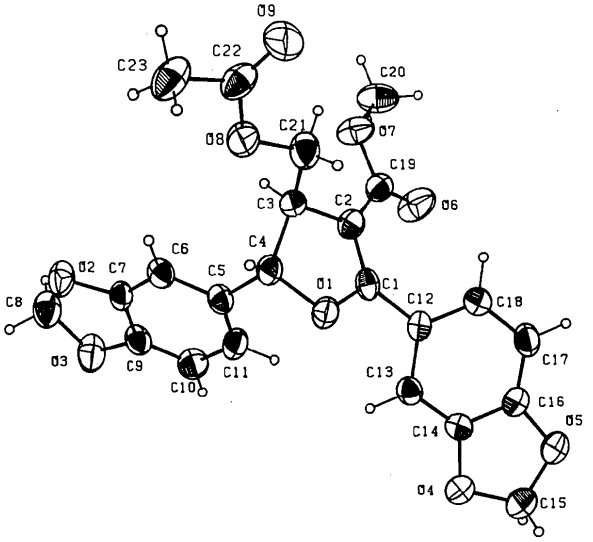

Fig. 1. Thermal-ellipsoid plot of the title compound showing the atom-numbering scheme. The H-atom radii are arbitrarily reduced.

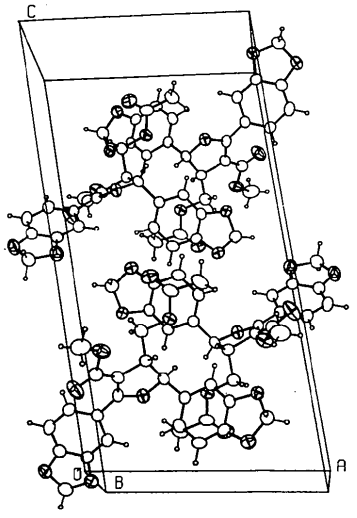

Fig. 2. Cell plot of the title dihydrofuran.

The ring geometry of this compound induces some internal bond angle compression for atoms C(1) through C(4). The bond angles 112·9 (4)° for O(1)–C(1)–C(2) and 109·1 (4)° for C(1)–C(2)–C(3) differ substantially from that normally associated with sp^2-hybridized carbon. As a result of this geometric angle compression, the angles C(2)–C(1)–C(12), C(1)–C(2)–C(19) and C(3)–C(2)–C(19) broaden to 134·8 (4), 127·0 (4) and 123·7 (4)°, respectively. Similarly at the sp^3-hybridized centers, the C(2)–C(3)–C(4) bond angle is 101·1 (3)° and the O(1)–C(4)–C(3) angle is 105·1 (3)°. The bond angle C(4)–C(3)–C(21) in turn broadens to 113·1 (4)°, the angle C(2)–C(3)–C(21) to 111·4 (4)° and bond angle C(3)–C(4)–C(5) to 112·7 (4)°. Bond lengths between atoms C(1) through C(4) are unaffected by ring geometry, however. The C(1)–C(2) bond length is 1·347 (6) Å, and the distances between C(2)–C(3) and C(3)–C(4) are 1·507 (5) and 1·536 (6) Å, respectively.

An analysis of the closest intermolecular contact distances reveals that van der Waals forces are likely to be a dominant stabilizing force in the crystal lattice. Several interactions were noted to occur with neighboring molecules. The hydrogen to non-hydrogen contact distance between H(2)C(8) and O(6) is 2·44 Å on a molecule related to that in Table 1 by $x-1, y, z$. The corresponding intermolecular C(8) to O(6) separation is 3·067 (6) Å. The H to H contact distance H(1)C(4) to H(1)C(3) on the same molecule at $1-x, y-\frac{1}{2}, \frac{1}{2}-z$ is 2·74 Å. The non-H to H contact distance from O(4) to H(2)C(15) at $-x, 1-y, -z$ is 2·53 Å, and the corresponding O(4) to C(15) internuclear separation is 3·293 (6) Å. For a molecule at $x-1, y+1, z$, the distance O(5) to H(1)C(8) is 2·74 Å, while the H to H contact distances H(2)C(15) to H(2)C(8) and H(2)C(15) to H(1)C(8) are both 2·87 Å. Other noticeably short non-H to H contact distances include O(9) to H(1)C(10) at 2·68 Å for a molecule at $x, -y-\frac{1}{2}, \frac{1}{2}+z$, and the O(4) to H(2)C(8) and O(9) to H(1)C(8) separations of 2·66 and 2·64 Å, respectively, with the neighboring molecules at $1-x, y, -z$ and $1-x, \frac{1}{2}+y, \frac{1}{2}-z$, respectively.

Intermolecular van der Waals interactions may prove to be important in the binding of an antagonist to the PAF-membrane receptor site. Additional investigations are now in progress in our laboratory to determine the utility of this X-ray crystallographic approach to the design of potent and specific antagonists and a drug-receptor site binding model.

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Structure of (±)-3-[1-Hydroxy-1-(4-methylphenyl)ethyl]-6-phenyl-1,2,4,5-tetrazine

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Abstract. $C_{17}H_{16}N_4O$, $M_r = 292{\cdot}34$, monoclinic, $C2/c$, $a = 22{\cdot}827\ (7)$, $b = 6{\cdot}004\ (4)$, $c = 23{\cdot}276\ (5)$ Å, $\beta = 108{\cdot}16\ (3)°$, $V = 3031{\cdot}3$ Å^3, $Z = 8$, $D_x = 1{\cdot}28$ g cm^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}71073$ Å, $\mu = 0{\cdot}8$ cm^{-1}, $F(000) = 1232$, $T = 294$ K, $R = 0{\cdot}063$ for 879 unique observed reflections. Bond lengths and angles lie within expected

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