

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å<sup>2</sup>)

$$B_{eq} = (8\pi^2/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	B <sub>eq</sub>
C1	0.2177 (6)	0.1990 (2)	0.9675 (4)	4.5 (1)
C2	0.1581 (5)	0.1276 (2)	0.8919 (3)	3.3 (1)
C3	-0.0271 (5)	0.1068 (2)	0.9404 (3)	3.5 (1)
O3	-0.1219 (4)	0.0500 (1)	0.9115 (2)	4.8 (1)
C4	-0.0628 (6)	0.1701 (2)	1.0257 (4)	4.8 (1)
C5	0.0699 (6)	0.1509 (3)	1.1339 (4)	5.4 (1)
C6	0.2610 (6)	0.1701 (3)	1.0925 (4)	5.6 (1)
C7	0.0330 (6)	0.2407 (2)	0.9750 (5)	5.2 (1)
O1'	0.1074 (3)	0.1548 (1)	0.7725 (2)	4.1 (1)
N2'	0.2302 (4)	0.1220 (2)	0.6976 (2)	3.6 (1)
C3'	0.3350 (4)	0.0724 (2)	0.7535 (3)	3.0 (1)
C4'	0.2960 (6)	0.0618 (2)	0.8772 (3)	4.3 (1)
C1''	0.4862 (4)	0.0354 (2)	0.6960 (3)	3.2 (1)
C2''	0.4858 (5)	-0.0446 (2)	0.6664 (3)	3.9 (1)
C3''	0.6290 (6)	-0.0791 (2)	0.6126 (4)	5.0 (1)
C4''	0.7786 (6)	-0.0334 (3)	0.5892 (4)	5.2 (1)
C5''	0.7853 (5)	0.0456 (3)	0.6174 (4)	4.8 (1)
C6''	0.6406 (4)	0.0788 (2)	0.6691 (3)	3.6 (1)
C12''	0.2979 (1)	-0.1021 (1)	0.6950 (1)	5.90 (3)
C16''	0.6527 (1)	0.1790 (1)	0.7034 (1)	5.84 (3)

Table 2. Selected geometric parameters (Å, °)

C1—C2	1.532 (5)	N2'—C3'	1.272 (4)
C1—C6	1.534 (6)	C3'—C4'	1.494 (5)
C1—C7	1.524 (6)	C3'—C1''	1.471 (5)
C2—C4'	1.516 (5)	C1''—C2''	1.396 (5)
C2—C3	1.541 (5)	C1''—C6''	1.397 (4)
C3—C4	1.494 (5)	C2''—C3''	1.385 (6)
C3—O3	1.212 (4)	C2''—C12''	1.730 (4)
C4—C5	1.549 (6)	C3''—C4''	1.379 (6)
C4—C7	1.524 (6)	C4''—C5''	1.375 (7)
C5—C6	1.540 (7)	C5''—C6''	1.373 (5)
O1'—N2'	1.409 (4)	C6''—C16''	1.741 (4)
O1'—C2	1.473 (4)		
C6—C1—C7	101.8 (3)	C2—O1'—N2'	109.5 (2)
C2—C1—C6	108.2 (3)	O1'—N2'—C3'	109.2 (2)
C2—C1—C7	100.9 (3)	N2'—C3'—C4'	114.4 (2)
C1—C2—C3	100.7 (3)	N2'—C3'—C1''	119.2 (2)
C1—C2—O1'	109.0 (2)	C4'—C3'—C1''	126.3 (3)
C1—C2—C4'	119.0 (3)	C2—C4'—C3'	101.5 (3)
C3—C2—O1'	104.9 (2)	C3'—C1''—C2''	122.5 (2)
C3—C2—C4'	118.6 (3)	C3'—C1''—C6''	121.4 (2)
O1'—C2—C4'	103.8 (2)	C2''—C1''—C6''	116.1 (2)
O3—C3—C4	128.6 (3)	C1''—C2''—C3''	122.2 (3)
C2—C3—O3	125.0 (3)	C1''—C2''—C12''	118.9 (2)
C2—C3—C4	106.4 (3)	C3''—C2''—C12''	118.9 (3)
C3—C4—C5	104.7 (3)	C2''—C3''—C4''	119.1 (3)
C3—C4—C7	101.3 (3)	C3''—C4''—C5''	120.7 (3)
C5—C4—C7	101.7 (3)	C4''—C5''—C6''	119.2 (3)
C4—C5—C6	102.7 (3)	C1''—C6''—C5''	122.7 (3)
C1—C6—C5	104.0 (3)	C1''—C6''—C16''	119.1 (2)
C1—C7—C4	95.3 (3)	C5''—C6''—C16''	118.1 (3)
C1—C2—C3—C4	5.5 (4)	C7—C1—C2—C3	-39.1 (4)
C2—C3—C4—C5	-75.5 (4)	C1—C2—C3—O3	-175.2 (3)
C3—C4—C5—C6	70.1 (4)	O1'—C2—C3—O3	71.7 (4)
C4—C5—C6—C1	0.8 (4)	C4'—C2—C1—C6	-64.0 (4)
C5—C6—C1—C2	-72.1 (4)	C1—C7—C4—C5	55.0 (4)
C6—C1—C2—C3	67.4 (4)	C7—C4—C5—C6	-35.1 (4)
C2—C3—C4—C7	29.9 (4)	C5—C6—C1—C7	33.7 (4)
C3—C4—C7—C1	-52.8 (4)	C6—C1—C7—C4	-54.4 (4)
C4—C7—C1—C2	57.1 (4)	C4'—C3'—C1''—C2''	73.3 (5)

Data collection: *AFC Software* (Rigaku Corporation, 1974). Cell refinement: *AFC Software*. Data reduction: *AFC Software*. Program(s) used to solve structure: *SHELX86* (Sheldrick, 1985). Program(s) used to refine structure: *SHELX76* (Sheldrick, 1976). Molecular graphics: *ORTEPII* (Johnson,

1976). Software used to prepare material for publication: *Xtal3.0* (Hall & Stewart, 1990). Calculations were performed on a VAX 8800 computer.

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: C940462-HR1029). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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## The Molecular Structure of Caroxazone, a Reversible Monoamine Oxidase Inhibitor

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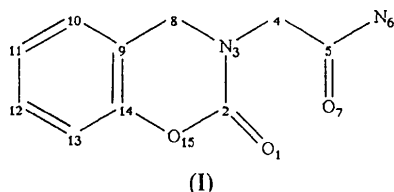
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### Abstract

Caroxazone, 2-oxo-2H-1,3-benzoxazine-3(4H)-acetamide (I), C<sub>10</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>, is a potent monoamine oxidase (MAO) inhibitor. The two molecules in the asymmetric unit have different conformations of the acetamide chain. The oxazine ring is not very distorted and the distances between the different atoms of the ring indicate electronic delocalization within this moiety. Crystal cohesion is assumed to be mainly due to intermolecular hydrogen bonding between the amidic N and carbonyl O atoms.

### Comment

As part of our study of monoamine oxidase (MAO) inhibitors (Moureau *et al.*, 1992; Wouters *et al.*, 1993; Wouters, Perpete, Norberg, Evrard & Durant, 1994), we report here the X-ray crystal structure of caroxazone, (I), a clinically active antidepressant drug (Moretti, Caccia, Carpentier & Carfagna, 1984). Crystal structure analysis of this compound has been undertaken in order to ascertain the conformation of the acetamide side chain with respect to the oxobenzoxazine moiety of the molecule; furthermore, the forces responsible for the crystal packing cohesion were examined in order to discover which functional groups of the caroxazone molecule are likely to interact with the MAO active site.



The two molecules of caroxazone in the asymmetric unit (numbered 100 and 200) adopt significantly different conformations. For both molecules, an 'enantiomeric' conformation is produced by symmetry (*a*

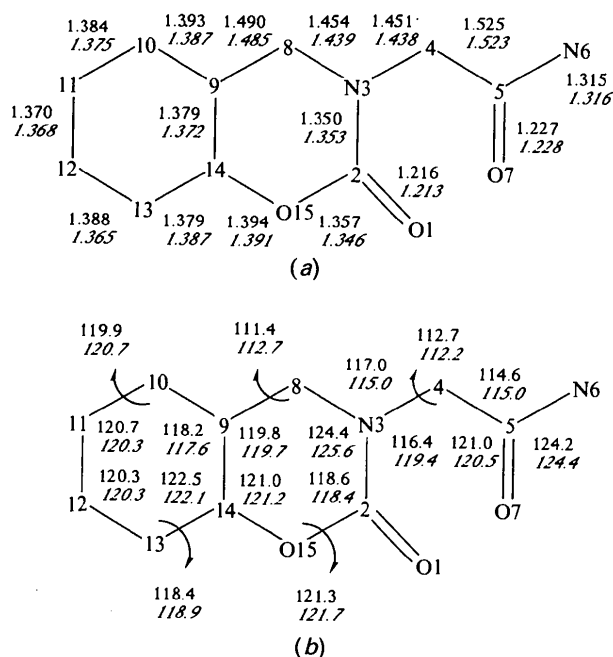


Fig. 1. Comparison of (a) the bond lengths (Å) and (b) the valence angles (°) of the two molecules of caroxazone; the atom labelling of the non-H atoms is included. The data for molecule 100 are shown in plain text and those for molecule 200 are shown in italic. The maximum e.s.d.'s are 0.006 Å and 0.3° for bonds and angles, respectively.

plane) leading to four stable conformations for the acetamide side chain of caroxazone. Implications of these steric requirements, with respect to the active site of MAO, will be discussed elsewhere.

Bond lengths and valence angles are compared in Fig. 1 and reported in Table 2. The main torsion angles are presented in Table 2. The oxazine ring is not very distorted (Table 2). The main deviations from the mean plane through atoms C02, N03, C08, C09, C14 and O15 are observed in the 100 molecule for the atoms N03 and C08, with out-of-plane distances of  $-0.111(2)$  and  $0.106(2)$  Å, respectively. In both molecules, the atom N03 retains its  $sp^2$  character as underlined by its small deviation from the mean plane defined by C02, C04 and C08, with distances of  $-0.120$  and  $-0.014$  Å in the 100 and 200 molecules, respectively, and by the sum of the valence angles at this N atom [ $357.8(2)$  and  $360.0(2)^\circ$  for the 100 and 200 molecules, respectively]. The C02—O15, C14—O15 and O01—C02 bond lengths (Fig. 1) fall between standard single- and double-bond lengths and indicate electronic delocalization within the oxobenzoxazine ring.

Crystal cohesion (Fig. 2) is assumed to be due to intermolecular hydrogen bonding between the amidic N atom (N06) and the carbonyl O atoms (O01 and O07) of two other molecules (Table 3). As a consequence, these functional groups (*i.e.* the amide of the acetamide chain and the carbonyl in the benzoxazine ring) are likely to anchor caroxazone to specific amino acids in the binding site of the enzyme.

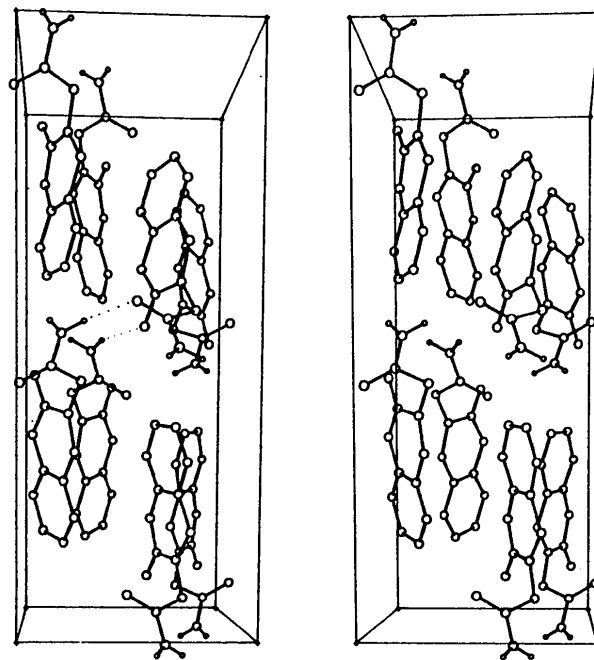


Fig. 2. Stereoview of the molecular conformation and crystal packing of caroxazone. Hydrogen bonds are represented by dotted lines.

**Experimental***Crystal data*C<sub>10</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub> $M_r = 206.20$ 

Orthorhombic

 $Pca2_1$  $a = 8.0934 (10) \text{ \AA}$  $b = 19.998 (3) \text{ \AA}$  $c = 11.926 (2) \text{ \AA}$  $V = 1930.2 (5) \text{ \AA}^3$  $Z = 8$  $D_x = 1.419 \text{ Mg m}^{-3}$ *Data collection*

Enraf–Nonius CAD-4

diffractometer

Absorption correction:

none

3289 measured reflections

1996 independent reflections

1747 observed reflections

 $[I > 2\sigma(I)]$ *Refinement*Refinement on  $F^2$  $R[F^2 > 2\sigma(F^2)] = 0.0357$  $wR(F^2) = 0.0852$  $S = 0.903$ 

1994 reflections

331 parameters

 $w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.0243P]$ where  $P = (F_o^2 + 2F_c^2)/3$ Cu  $K\alpha$  radiation $\lambda = 1.54178 \text{ \AA}$ 

Cell parameters from 25

reflections

 $\theta = 14\text{--}28^\circ$  $\mu = 0.897 \text{ mm}^{-1}$  $T = 293 (2) \text{ K}$ 

Prism

 $0.31 \times 0.22 \times 0.05 \text{ mm}$ 

Colourless

 $R_{\text{int}} = 0.0191$  $\theta_{\text{max}} = 71.89^\circ$  $h = 0 \rightarrow 9$  $k = -24 \rightarrow 21$  $l = 0 \rightarrow 14$ 

3 standard reflections

frequency: 60 min

intensity variation: none

 $(\Delta/\sigma)_{\text{max}} = 1.457$  $\Delta\rho_{\text{max}} = 0.12 \text{ e \AA}^{-3}$  $\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$ 

Atomic scattering factors

from *International Tables for Crystallography* (1992),

Vol. C, Tables 4.2.6.8 and 6.1.1.4)

C212	0.1128 (5)	0.63274 (15)	0.5543 (3)	0.0623 (11)
C213	0.0804 (4)	0.68783 (16)	0.4904 (3)	0.0540 (9)
C214	0.1323 (3)	0.74995 (13)	0.5283 (2)	0.0431 (7)

Table 2. Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

O101—C102	1.216 (3)	O201—C202	1.213 (4)
O107—C105	1.227 (3)	O207—C205	1.228 (3)
O115—C102	1.357 (3)	O215—C202	1.346 (4)
O115—C114	1.394 (3)	O215—C214	1.391 (3)
N103—C102	1.350 (3)	N203—C202	1.353 (4)
N103—C104	1.451 (4)	N203—C204	1.438 (4)
N103—C108	1.454 (3)	N203—C208	1.439 (4)
N106—C105	1.313 (3)	N206—C205	1.316 (4)
C104—C105	1.525 (4)	C204—C205	1.523 (5)
C108—C109	1.490 (4)	C208—C209	1.485 (4)
C109—C110	1.393 (4)	C209—C210	1.387 (4)
C109—C114	1.379 (3)	C209—C214	1.372 (3)
C110—C111	1.384 (5)	C210—C211	1.375 (4)
C111—C112	1.370 (6)	C211—C212	1.368 (5)
C112—C113	1.388 (5)	C212—C213	1.365 (5)
C113—C114	1.379 (4)	C213—C214	1.387 (4)
C102—O115—C114	121.3 (2)	C202—O215—C214	121.7 (2)
C102—N103—C104	116.4 (2)	C202—N203—C204	119.4 (3)
C102—N103—C108	124.4 (2)	C202—N203—C208	125.6 (2)
C104—N103—C108	117.0 (2)	C204—N203—C208	115.0 (3)
O101—C102—O115	117.6 (2)	O201—C202—O215	117.6 (3)
O101—C102—N103	123.7 (2)	O201—C202—N203	123.9 (3)
O115—C102—N103	118.6 (2)	O215—C202—N203	118.4 (3)
N103—C104—C105	112.7 (2)	N203—C204—C205	112.2 (3)
O107—C105—N106	124.4 (2)	O207—C205—N206	124.4 (3)
O107—C105—C104	121.0 (2)	O207—C205—C204	120.4 (3)
N106—C105—C104	114.6 (2)	N206—C205—C204	115.0 (2)
N103—C108—C109	111.4 (2)	N203—C208—C209	112.7 (3)
C108—C109—C110	122.0 (2)	C208—C209—C210	122.6 (3)
C108—C109—C114	119.8 (2)	C208—C209—C214	119.7 (2)
C110—C109—C114	118.2 (3)	C210—C209—C214	117.6 (2)
C109—C110—C111	119.9 (3)	C209—C210—C211	120.7 (3)
C110—C111—C112	120.7 (3)	C210—C211—C212	120.3 (3)
C111—C112—C113	120.3 (3)	C211—C212—C213	120.3 (3)
C112—C113—C114	118.4 (3)	C212—C213—C214	118.9 (3)
O115—C114—C109	121.0 (2)	O215—C214—C209	121.2 (2)
O115—C114—C113	116.5 (2)	O215—C214—C213	116.7 (2)
C109—C114—C113	122.5 (3)	C209—C214—C213	122.1 (3)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j$$

	$x$	$y$	$z$	$U_{\text{eq}}$
O101	0.0596 (3)	0.45533 (10)	0.5469 (2)	0.0600 (7)
O107	0.0030 (2)	0.43034 (9)	0.8109 (2)	0.0502 (6)
O115	0.0484 (2)	0.34889 (9)	0.50010 (17)	0.0526 (6)
N103	0.2126 (2)	0.38310 (10)	0.64972 (18)	0.0415 (6)
N106	0.1785 (3)	0.51049 (12)	0.8679 (2)	0.0516 (8)
C102	0.1055 (3)	0.39867 (13)	0.5670 (2)	0.0458 (8)
C104	0.2671 (3)	0.43790 (12)	0.7203 (3)	0.0453 (8)
C105	0.1362 (3)	0.45942 (11)	0.8049 (2)	0.0379 (7)
C108	0.2411 (4)	0.31573 (12)	0.6912 (2)	0.0460 (8)
C109	0.1925 (3)	0.26450 (13)	0.6067 (2)	0.0439 (8)
C110	0.2406 (5)	0.19787 (13)	0.6161 (3)	0.0591 (10)
C111	0.1927 (5)	0.15205 (16)	0.5354 (4)	0.0726 (13)
C112	0.0968 (5)	0.17135 (18)	0.4464 (3)	0.0729 (11)
C113	0.0503 (4)	0.23774 (17)	0.4342 (3)	0.0593 (10)
C114	0.0997 (3)	0.28295 (14)	0.5148 (2)	0.0446 (8)
O201	0.0900 (3)	0.91217 (13)	0.4286 (3)	0.0853 (10)
O207	−0.0244 (2)	0.93474 (9)	0.7253 (2)	0.0628 (7)
O215	0.1022 (3)	0.80417 (10)	0.45814 (18)	0.0591 (7)
N203	0.2082 (3)	0.87741 (10)	0.5906 (2)	0.0500 (7)
N206	0.1426 (3)	1.02019 (13)	0.7729 (3)	0.0629 (10)
C202	0.1313 (4)	0.86743 (14)	0.4913 (3)	0.0534 (9)
C204	0.2345 (5)	0.94455 (14)	0.6299 (4)	0.0645 (10)
C205	0.1060 (3)	0.96569 (12)	0.7162 (3)	0.0493 (8)
C208	0.2637 (5)	0.82571 (14)	0.6656 (3)	0.0550 (9)
C209	0.2126 (3)	0.75786 (12)	0.6287 (2)	0.0418 (7)
C210	0.2424 (4)	0.70097 (14)	0.6921 (3)	0.0556 (9)
C211	0.1945 (4)	0.63901 (16)	0.6542 (3)	0.0660 (11)

C114—O115—C102—O101	177.6 (2)
C114—O115—C102—N103	−0.7 (3)
C102—O115—C114—C109	8.8 (3)
C102—O115—C114—C113	−172.3 (2)
C104—N103—C102—O101	3.1 (4)
C108—N103—C102—O101	165.8 (3)
C104—N103—C102—O115	−178.7 (2)
C108—N103—C102—O115	−16.0 (3)
C102—N103—C104—C105	76.0 (3)
C108—N103—C104—C105	−88.0 (3)
C104—N103—C108—C109	−175.2 (2)
C102—N103—C108—C109	22.2 (3)
N103—C104—C105—N106	−177.7 (2)
N103—C104—C105—O107	1.9 (4)
N103—C108—C109—C110	165.7 (3)
N103—C108—C109—C114	−13.1 (3)
C108—C109—C110—C111	−179.9 (3)
C114—C109—C110—C111	−1.1 (5)
C108—C109—C114—O115	−0.8 (4)
C108—C109—C114—C113	−179.6 (3)
C110—C109—C114—O115	−179.6 (3)
C110—C109—C114—C113	1.5 (4)
C109—C110—C111—C112	−0.6 (6)
C110—C111—C112—C113	1.9 (6)
C111—C112—C113—C114	−1.5 (5)
C112—C113—C114—O115	−179.1 (3)
C112—C113—C114—C109	−0.3 (5)
C214—O215—C202—O201	−174.4 (3)
C214—O215—C202—N203	7.2 (4)
C202—O215—C214—C209	−8.5 (4)
C202—O215—C214—C213	172.9 (3)
C204—N203—C202—O201	4.3 (5)

C208—N203—C202—O201	-177.9 (3)
C204—N203—C202—O215	-177.5 (3)
C208—N203—C202—O215	0.3 (5)
C202—N203—C204—C205	99.5 (4)
C208—N203—C204—C205	-78.5 (4)
C204—N203—C208—C209	171.9 (3)
C202—N203—C208—C209	-5.9 (5)
N203—C204—C205—N206	166.0 (3)
N203—C204—C205—O207	-17.6 (5)
N203—C208—C209—C210	-175.4 (3)
N203—C208—C209—C214	4.5 (4)
C208—C209—C210—C211	-179.3 (3)
C214—C209—C210—C211	0.8 (4)
C208—C209—C214—O215	2.1 (4)
C208—C209—C214—C213	-179.3 (3)
C210—C209—C214—O215	-178.0 (2)
C210—C209—C214—C213	0.6 (4)
C209—C210—C211—C212	-1.6 (5)
C210—C211—C212—C213	1.1 (5)
C211—C212—C213—C214	0.3 (6)
C212—C213—C214—O215	177.5 (3)
C212—C213—C214—C209	-1.1 (5)

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

D—H...A	H...A	D—H...A
N106—H161...O107 <sup>i</sup>	2.104 (48)	166.4 (45)
N106—H162...O101 <sup>ii</sup>	2.162 (46)	167.0 (37)
N206—H261...O207 <sup>iii</sup>	2.032 (48)	166.2 (37)
N206—H262...O201 <sup>iv</sup>	1.978 (44)	163.0 (35)

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

The structure was solved using *SHELXS86* (Sheldrick, 1990) and refined with *SHELXL93* (Sheldrick, 1993). Most of the calculations were performed with the *SHELXL93* package, as was the generation of the Crystallographic Information File (CIF) used for the submission of this paper.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and torsion angles have been deposited with the IUCr (Reference: DU1075). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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## 3-[5-(2-Nitrophenyl)furfurylidene]-2,4-pentanedione

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## Abstract

The title compound,  $C_{16}H_{13}NO_5$ , consists of monomeric units. The whole molecule was tested for planarity. Unlike the 3-nitrophenyl isomer [Lokaj, Vrabel, Sivý, Ilavský & Koreňová (1994). *Acta Cryst.* **C50**, 1312–1314], the fragment containing the O(1), C(1), C(2) and C(5) atoms, the furylidene ring and the attached nitrophenyl group are not in the same plane. The dihedral angle between the benzene and furan rings is 47.8°.

## Comment

The conformation of furan derivatives with an *R* substituent at position 5 and a  $—CH=CR'_2$  substituent at position 2 can be assumed on the basis of previously reported information (Kusá, Polynova, Poray-Koshits, Kováč & Végh, 1979; Kusá, Polynova, Poray-Koshits & Jurášek, 1979; Kusá, Polynova, Poray-Koshits & Kováč, 1979). The conformation depends on the type of *R'* substituent; electron-acceptor substituents form *trans* and