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Methyl 3-dimethylamino-2-(2-{2-dimethylamino-1-[3-(3-pyridyl)-1,2,4-oxadiazol-5-yl]vinyloxy}-phenyl)acrylate

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Key indicators

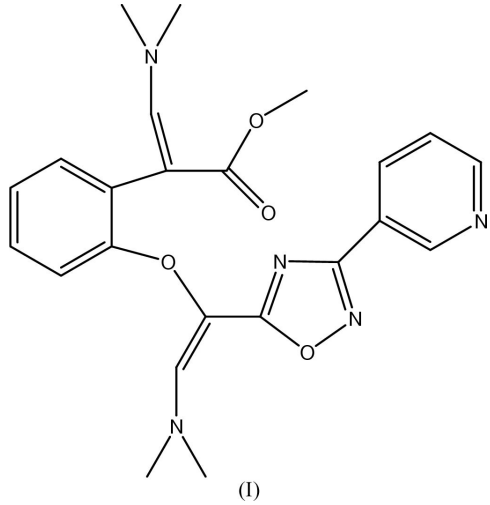
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.053
wR factor = 0.182
Data-to-parameter ratio = 14.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{23}H_{25}N_5O_4$, was synthesized by the reaction of methyl (2-{[3-(3-pyridyl)-1,2,4-oxadiazol-5-yl]-methoxy}phenyl)acetate and *N*,*N*-dimethylformamide dimethyl acetal. In the crystal structure, there are intramolecular C—H···O and C—H···N and intermolecular C—H···π interactions.

Comment

1,2,4-Oxadiazoles represent an important class of five-membered heterocycles. The derivatives of 1,2,4-oxadiazoles have intrinsic analgesic (Terashita *et al.*, 2002), *anti*-inflammatory (Nicolaides *et al.*, 1998) and antipicornaviral (Romero, 2001) properties. They are known as agonists [for angiotension (Naka & Kubo, 1999) and adhesion promoters (Juraszyk *et al.*, 1997)] for different receptors. We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) (Fig. 1) shows normal bond lengths and angles (Table 1), and weak intramolecular C—H···O and C—H···N hydrogen bonds (Table 2). There are also intermolecular C—H···π interactions (Fig. 2), involving the benzene and pyridine rings (Table 2). These weak interactions stabilize the crystal structure.

Experimental

Methyl (2-{[3-(3-pyridyl)-1,2,4-oxadiazol-5-yl]methoxy}phenyl)acetate (14 mmol) was dissolved in dimethylformamide (20 ml) and *N*,*N*-dimethylformamide dimethyl acetal (8 ml) was added in one portion. The resulting mixture was refluxed for 10 h, then concentrated under reduced pressure to afford crude compound (I). Pure compound (I) was obtained by crystallization from a mixture of ethyl acetate

(15 ml) and petroleum ether (7.5 ml). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution. ^{1}H NMR ($CDCl_3$): δ 9.19 (*m*, 1H), 8.67–8.68 (*m*, 1H), 8.24–8.26 (*m*, 1H), 7.70 (*m*, 1H), 7.35 (*m*, 2H), 7.18–7.20 (*m*, 2H), 6.96 (*m*, 1H), 6.88–6.89 (*m*, 1H), 3.56 (*s*, 3H), 3.03 (*m*, 6H), 2.86–2.89 (*s*, 6H).

Crystal data

$C_{23}H_{25}N_5O_4$
M_r = 435.48
Monoclinic, $P2_1/c$
a = 8.6250 (17) Å
b = 9.6390 (19) Å
c = 26.273 (5) Å
β = 91.28 (3)°
V = 2183.7 (8) Å^3
Z = 4
D_x = 1.325 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10–13°
μ = 0.09 mm^{-1}
T = 293 (2) K
Tablet, colourless
0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.964, T_{max} = 0.982
4550 measured reflections
4257 independent reflections
2426 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 26.0°
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 11$
$l = -31 \rightarrow 31$
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.182
S = 0.93
4257 reflections
290 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 1.2P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.013
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0100 (17)

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.350 (3)	N4—C22	1.445 (4)
O1—N2	1.425 (3)	N4—C23	1.456 (4)
O2—C9	1.399 (3)	N5—C18	1.342 (4)
O2—C8	1.394 (3)	N5—C20	1.444 (4)
O3—C16	1.208 (4)	N5—C19	1.453 (4)
O4—C16	1.352 (4)	C4—C6	1.470 (4)
O4—C17	1.441 (4)	C7—C8	1.440 (4)
N2—C6	1.291 (4)	C8—C21	1.348 (4)
N3—C7	1.301 (4)	C14—C15	1.487 (4)
N3—C6	1.383 (4)	C15—C18	1.355 (4)
N4—C21	1.342 (4)	C15—C16	1.458 (4)
C7—O1—N2	105.9 (2)	N2—C6—N3	115.7 (3)
C9—O2—C8	117.8 (2)	N2—C6—C4	120.9 (3)
C16—O4—C17	116.2 (3)	N3—C6—C4	123.4 (3)
C5—N1—C1	115.8 (3)	N3—C7—O1	113.4 (2)
C6—N2—O1	103.0 (2)	N3—C7—C8	128.8 (3)
C7—N3—C6	102.0 (2)	O1—C7—C8	117.8 (2)
C21—N4—C22	124.7 (3)	C21—C8—O2	124.4 (3)
C21—N4—C23	120.0 (3)	C21—C8—C7	120.7 (3)
C22—N4—C23	115.3 (3)	O2—C8—C7	114.8 (2)
C18—N5—C20	120.0 (3)	C10—C9—O2	123.1 (2)
C18—N5—C19	124.0 (3)	C14—C9—O2	115.0 (2)
C20—N5—C19	116.0 (3)	C18—C15—C16	114.4 (3)
N1—C1—C2	124.4 (3)	C18—C15—C14	126.8 (3)
C1—C2—C3	118.9 (3)	C16—C15—C14	118.6 (2)
C2—C3—C4	118.4 (3)	O3—C16—O4	121.6 (3)
C5—C4—C3	117.8 (3)	O3—C16—C15	126.9 (3)
C5—C4—C6	120.8 (3)	O4—C16—C15	111.5 (3)
C3—C4—C6	121.3 (3)	N4—C21—C8	131.6 (3)
N1—C5—C4	124.6 (3)		

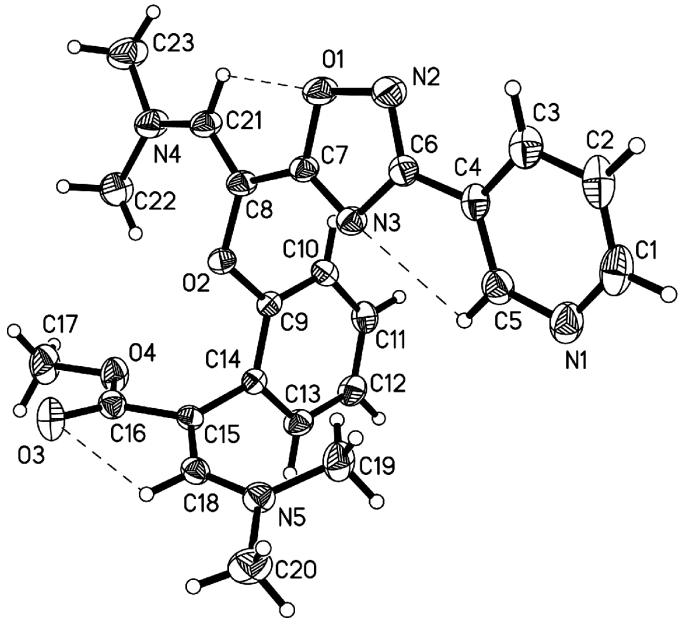


Figure 1
View of (I), showing displacement ellipsoids drawn at the 30% probability level. Dashed lines indicate C—H···O and C—H···N hydrogen bonds.

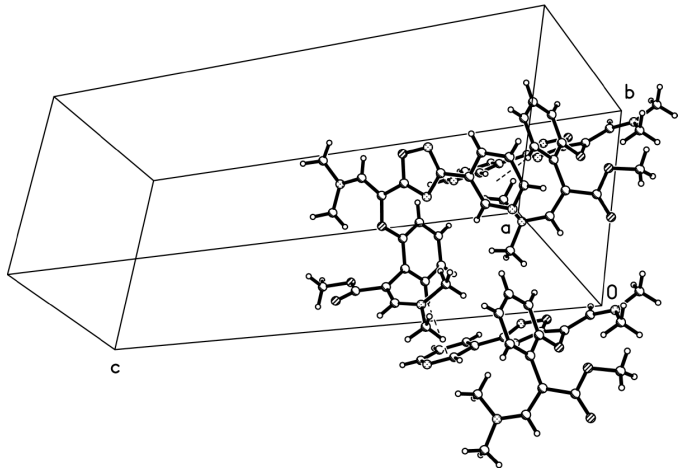


Figure 2
Part of the crystal packing of (I). The intermolecular C—H···π interactions are indicated by dashed lines.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5A···N3	0.93	2.60	2.944 (4)	103
C18—H18A···O3	0.93	2.38	2.778 (4)	105
C21—H21A···O1	0.93	2.34	2.758 (3)	107
C13—H13A···$Cg1^{i}$	0.93	2.58	3.488 (2)	164

Symmetry code: (i) $-x, y-\frac{1}{2}, \frac{1}{2}-z$. $Cg1$ is the centroid of the N1/C1–C5 ring.

All H atoms were positioned geometrically at distances of 0.93–0.96 Å and included in the refinement in riding-model approximation, with U_{iso}(H) = 1.2 or 1.5U_{eq} of the carrier atom.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

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