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

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.060
wR factor = 0.196
Data-to-parameter ratio = 14.9

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

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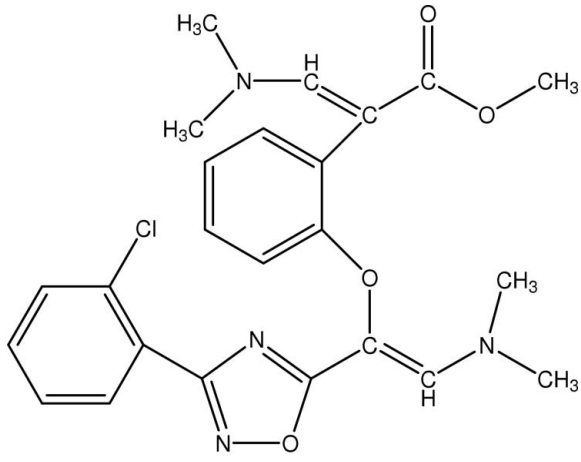
The title compound, $C_{24}H_{25}ClN_4O_4$, was synthesized by the reaction of methyl 2-{[3-(2-chlorophenyl)-1,2,4-oxadiazol-5-yl]methoxy}phenylacetate and *N*,*N*-dimethylformamide dimethyl acetal. There are short intramolecular C—H···O contacts in the molecule.

Comment

1,2,4-Oxadiazoles are an important class of five-membered heterocycles. Some derivatives of 1,2,4-oxadiazoles have intrinsic analgesic (Terashita *et al.*, 2002), anti-inflammatory (Nicolaides *et al.*, 1998) and antipicornaviral (Romero, 2001) properties, and also function as agonists (*e.g.* for angiotensin; Naka & Kubo, 1999) and antagonists (Juraszyk *et al.*, 1997) for different cellular adhesion receptors. We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) involves short intramolecular C—H···O contacts (Table 1), as shown in Fig. 1. Bond lengths and angles are unexceptional. The C7–C12 and C19–C24 benzene rings form dihedral angles of 100.6 and 47.6°, respectively, with the oxadiazole ring.

Experimental

Methyl 2-{[3-(2-chlorophenyl)-1,2,4-oxadiazol-5-yl]methoxy}phenylacetate (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 6 h, then concentrated under reduced pressure to afford crude (I). Pure (I) was obtained by recrystallizing from 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,

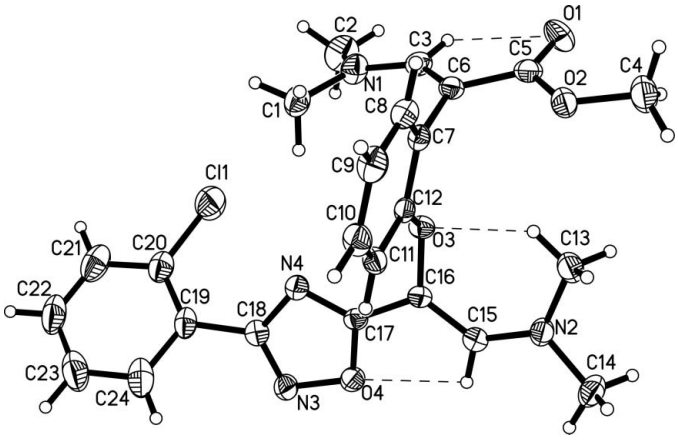


Figure 1
A view of the molecular structure of (I), with dashed lines indicating short intramolecular C—H···O contacts. Displacement ellipsoids are drawn at the 30% probability level

p.p.m.): 7.77–7.79 (*m*, 1H), 7.68 (*s*, 1H), 7.46–7.48 (*m*, 1H), 7.34–38 (*m*, 1H), 7.29–7.32 (*m*, 2H), 7.17–7.20 (*m*, 2H), 6.93–6.97 (*m*, 1H), 6.89–6.91 (*m*, 1H), 3.55 (**s**, 3H), 3.01 (***s***, 6H), 2.82 (***s***, 6H).

Crystal data

$C_{24}H_{25}ClN_4O_4$
M_r = 468.93
Monoclinic, $P2_1/c$
a = 16.088 (3) Å
b = 8.3060 (17) Å
c = 17.358 (4) Å
β = 95.79 (3)°
V = 2307.7 (8) Å^3
Z = 4
D_x = 1.350 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 9–12°
μ = 0.20 mm^{-1}
T = 293 (2) K
Block, colourless
0.4 × 0.3 × 0.2 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
4653 measured reflections
4491 independent reflections
2364 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 26.0°
$h = 0 \rightarrow 19$
$k = 0 \rightarrow 9$
$l = -20 \rightarrow 20$
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.196
S = 1.02
4491 reflections
301 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.9P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.91 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3A···O1	0.93	2.33	2.750 (4)	107
C13—H13A···O3	0.96	2.20	2.962 (4)	136
C15—H15A···O4	0.93	2.38	2.793 (4)	107

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