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(5-Methylisoxazol-3-yl)[2-(5-methylisoxazol-3-yl)-2,3-dihydro-1H-isoindol-1-ylidene]amine

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Key indicators

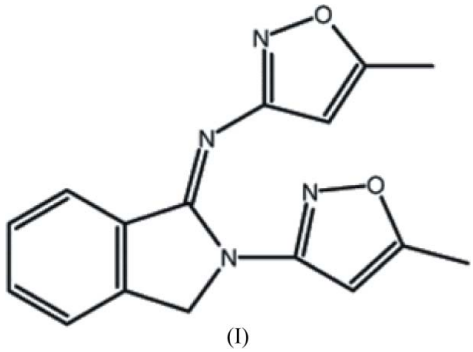
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.121
Data-to-parameter ratio = 13.9

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

The title compound, $C_{16}H_{14}N_4O_2$, was synthesized by the reaction of *o*-phthalaldehyde and 5-methyl-4,5-dihydroisoxazol-3-ylamine in dichloromethane. The conformation of the molecular structure may be influenced by a weak intramolecular C—H···N interaction and weak C—H···π interactions, and π–π stacking interactions may influence the crystal packing.

Comment

A large number of isoindoline derivatives such as staurosporine, indoprofen, and pazinaclone have been reported to possess biological activities (Takahashi & Hatanaka, 1997; Kundu *et al.*, 2001; Olmo *et al.*, 2003; Takahashi *et al.*, 2004; Cul *et al.*, 2004). Compound (I) shows antifungal activity against four species: *Chrysoporium tropicum*, *Fusarium oxysporum*, *Geotrichum candidum* and *Trichoplyton rubrum* (Al-Shihry, 2005).



(I)

The molecular structure of (I) is shown in Fig. 1. All geometric parameters are in normal ranges (Allen *et al.*, 1987). Each of the individual rings is essentially planar. The isoindole system *A* (N1/C1–C8) is almost planar, with maximum deviations of −0.020 (2), 0.027 (2) and −0.024 (1)Å for atoms C5, C7 and C8, respectively. The five-membered isoxazole rings *B* (O1/N2/C9–C11) and *C* (O2/N4/C13–C15) make a dihedral angle of 75.35 (9)° with one another. The dihedral angles between rings *A*/*B* and *A*/*C* are 2.72 (7) and 76.59 (7)°, respectively. A weak intramolecular C—H···N hydrogen bond (Table 1) may influence the conformation of the molecular structure.

A packing diagram of (I) is shown in Fig. 2. In the crystal structure, significant π–π stacking interactions exist between five-membered rings, where $Cg1\cdots Cg3(1-x, 1-y, 1-z)$ = 3.6285 (9) Å (*Cg*1 and *Cg*3 are the centroids of atoms O1/N2/C9–C11 and N1/C1/C6–C8) and the perpendicular distance is 3.49 (9) Å. These and three weak intermolecular C—H···π(arene) interactions may influence the crystal packing.

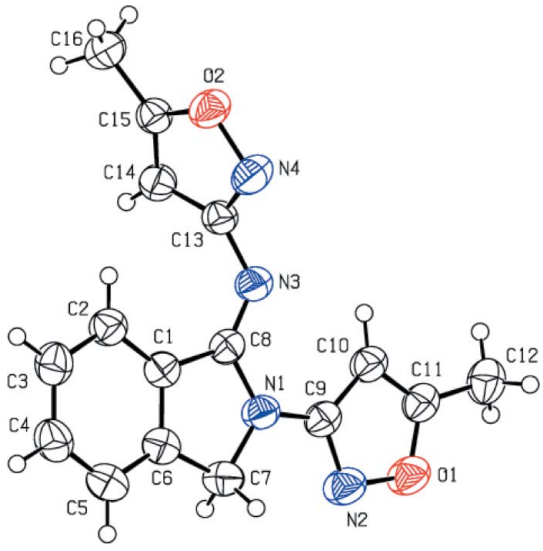


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and H atoms drawn as small spheres.

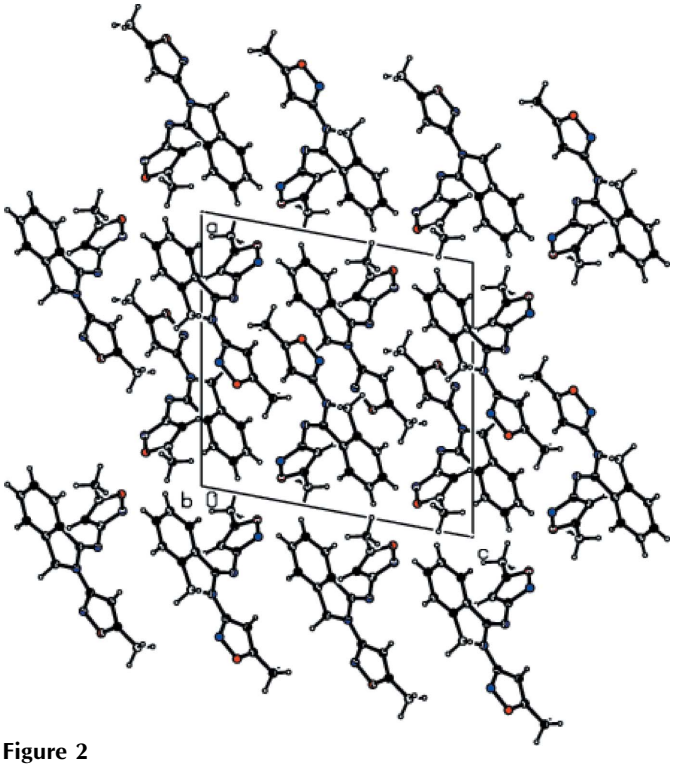


Figure 2
A view of the packing of (I).

Experimental

Compound (I) was obtained by the reaction of a stirred solution of *o*-phthalaldehyde (0.5 g, 3.73 mmol) in dichloromethane (20 ml) with a solution of 5-methyl-4,5-dihydroisoxazol-3-ylamine (0.73 g, 7.44 mmol) in dichloromethane (20 ml) (Al-Shihry, 2005). Yellow single crystals of (I) suitable for X-ray crystallographic analysis were obtained by slow evaporation of the reaction mixture (yield: 0.75 g, 68%; m.p. 464 K).

Crystal data

$C_{16}H_{14}N_4O_2$
M_r = 294.31
Monoclinic, $P2_1/c$
a = 13.5698 (8) Å
b = 7.8257 (6) Å
c = 13.6527 (8) Å
β = 100.690 (4)°
V = 1424.66 (16) Å^3
Z = 4
D_x = 1.372 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
Prism with corners rounded, colorless
0.44 × 0.36 × 0.29 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.960, T_{max} = 0.973
11079 measured reflections
2807 independent reflections
2318 reflections with $I > 2\sigma(I)$
R_{int} = 0.095
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.121
S = 1.07
2807 reflections
202 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0573P)^2 + 0.1431P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.026 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···N3	0.93	2.48	2.920 (2)	109
C2—H2···*Cg*2	0.93	2.88	3.6348 (17)	139
C12—H12*A*···*Cg*4^{i}	0.96	2.96	3.5516 (18)	121
C16—H16*B*···*Cg*4^{ii}	0.96	2.74	3.5597 (18)	144

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, y-1, z$. *Cg*2 and *Cg*4 are the centroids of atoms O2/N4/C13–C15 and C1–C6, respectively.

H atoms were placed in calculated positions and refined as riding on their parent atoms, with C—H = 0.96 (CH_3), 0.97 (CH_2) or 0.93Å (CH), and with U_{iso}(H) = 1.5U_{eq}(CH_3) or 1.2U_{eq}(CH_2,CH).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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