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1-[(*E*)-(3,4-Dimethylisoxazol-5-yl)iminomethyl]-2-naphthol

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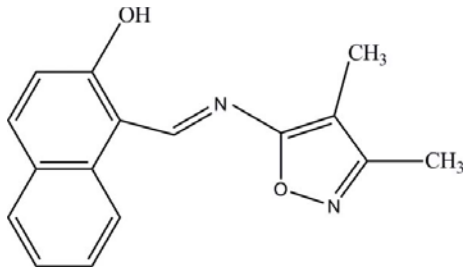
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.134; data-to-parameter ratio = 15.6.

The title Schiff base compound, $C_{16}H_{14}N_2O_2$, has been synthesized by the reaction of 5-amino-3,4-dimethylisoxazole and 2-hydroxy-1-naphthaldehyde. The dihedral angle between the isoxazole ring and the napthyl ring system is 3.29 (7)°. The molecule adopts an *E* configuration about the central C=N double bond. Intramolecular O—H···N hydrogen bonding generates an *S*(6) ring motif. In the crystal structure, π–π interactions are observed involving the isoxazole ring and the substituted benzene ring of the naphthyl unit, with centroid–centroid distances of 3.5200 (10) Å.

Related literature

For related background and the biological activity of isoxazol, see: Howell & Kimmel (2008); Bartlett & Schleyerbach (1985); Lamani *et al.* (2009); Jayashankar *et al.* (2009). For related structures, see: Alvarez-Thon *et al.* (2006); Tahir *et al.* (2008); Shad *et al.* (2008); Fun *et al.* (2010). For details of hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



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Experimental

Crystal data

$C_{16}H_{14}N_2O_2$
M_r = 266.29
Monoclinic, $P2_1/c$
a = 7.5250 (6) Å
b = 15.4643 (12) Å
c = 12.3982 (7) Å
β = 117.377 (4)°
V = 1281.17 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.79 × 0.06 × 0.05 mm

Data collection

Bruker APEX DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.930, T_{max} = 0.996
16577 measured reflections
3704 independent reflections
2843 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.134
S = 1.05
3704 reflections
237 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*1···N1	0.97 (2)	1.66 (3)	2.5471 (15)	150 (2)

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2761).

References

Alvarez-Thon, L., Bustos, C., Schott, E., Sanchez, C. & Ibañez, A. (2006). *Acta Cryst.* E**62**, o595–o597.
Bartlett, R. R. & Schleyerbach, R. (1985). *Int. J. Immunopharmacol.* **7**, 7–18.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
Fun, H.-K., Hemamalini, M., Asiri, A. M., Khan, S. A. & Khan, K. A. (2010). *Acta Cryst.* E**66**, o773–o774.
Howell, L. L. & Kimmel, H. L. (2008). *Biochem. Pharmacol.* **75**, 196–217.
Jayashankar, B., Rai, K. M. L., Baskaran, N. & Sathish, H. S. (2009). *Eur. J. Med. Chem.* **44**, 3898–3902.