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(2*E*,3*E*)-Ethyl 2-[(naphthalen-8-ylamino)methylene]-3-(naphthalen-1-ylimino)butanoate

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.056
wR factor = 0.175
Data-to-parameter ratio = 17.3

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

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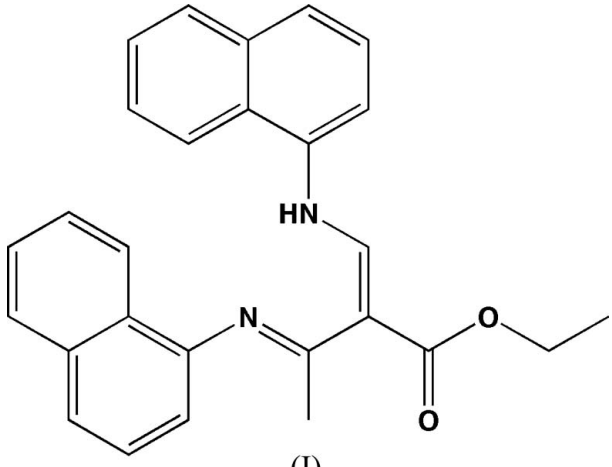
The title compound, $C_{27}H_{24}N_2O_2$, is built up from an unsaturated ester attached to two naphthylamine fragments. An intramolecular N—H···N hydrogen bond may influence the conformation of the molecule.

Comment

The biological and pharmaceutical importance of quinoline and benzoquinoline derivatives is of growing interest (Kerry *et al.*, 1999). Their antimalarial properties confer on them a recognized medicinal application (Narine & Meth-Cohn, 1979; Kraak *et al.*, 1997; Moussoui *et al.*, 2002).



(I)

Our group recently reported the structures of 2-chloro-3-chloromethylbenzo[*h*]quinoline (Beghidja *et al.*, 2004) and 2-methyl-3-ethyl methanoate benzo[*h*]quinoline (Benboudiaf *et al.*, 2005) obtained using the Vilsmeir method (Meth-Cohn *et al.*, 1981). During the preparation of this last derivative, a second compound, (I), was isolated; its structure is reported here.

The structure of (I) is built up from an unsaturated ester attached to two naphthylamine fragments (Fig. 1). The two naphthalene systems make a planar and make a dihedral angle of 71.44 (1)°. Bond distances and angles are within expected ranges and comparable with those for related compounds. There is an intramolecular N—H···N hydrogen bond (Table 1) which may influence the conformation of the molecule.

Experimental

At a temperature ranging between 273 and 278 K, phosphorus oxychloride ($POCl_3$, 0.015 mol) was added dropwise to dry dimethylformamide (DMF, 0.015 mol). Stirring was continued for

30 min, then a solution of (*E*)-ethyl 3-(naphthalen-8-ylamino)but-2-enoate (0.05 mol) in purified chloroform (25 ml) was added. The resulting mixture was stirred at 273 K for 2 h and then allowed to stand at room temperature before being transferred to a saturated $NaHCO_3$ aqueous solution. The organic layer was extracted with chloroform and dried with anhydrous magnesium sulfate. After evaporation of the CH_3Cl *in vacuo* overnight, a yellow solid residue was obtained. Yellow needle-shaped crystals of (I) were obtained by slow evaporation.

Crystal data

$C_{27}H_{24}N_2O_2$
M_r = 408.48
Monoclinic, $P2_1/c$
a = 6.9502 (5) Å
b = 16.2139 (7) Å
c = 19.2198 (7) Å
β = 95.309 (2)°
V = 2156.6 (2) Å^3
Z = 4
D_x = 1.258 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 173 (2) K
Needle, yellow
0.3 × 0.2 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer
φ scans, and ω scans with κ offsets
Absorption correction: none
8395 measured reflections
4889 independent reflections
2750 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 27.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.175
S = 1.02
4889 reflections
282 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0813P)^2 + 0.2247P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2	0.86	1.95	2.596 (2)	131

All H atoms were positioned geometrically and treated as riding, with C—H = 0.93 (CH), 0.97 (methylene) or 0.96 Å (CH_3) and N—H = 0.86 Å, with U_{iso}(H) = 1.2U_{eq}(CH, CH_2 or N) and 1.5U_{eq}(CH_3).

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Nonius, 1998); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

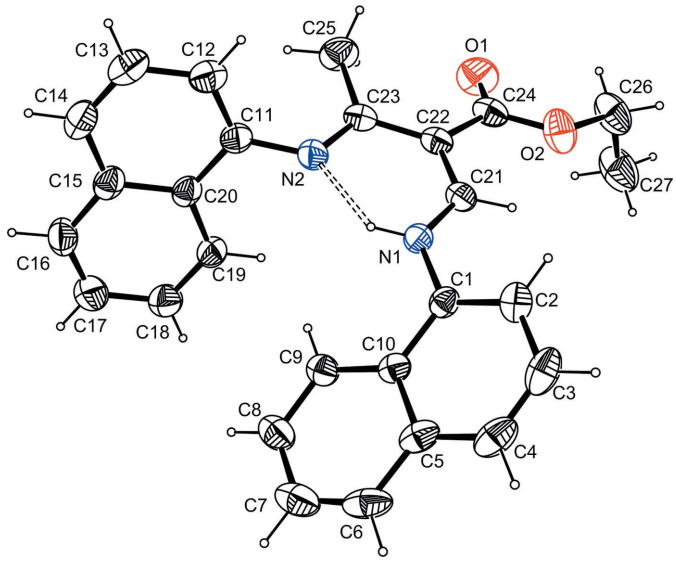


Figure 1
The molecular structure of the title compound, showing the atomic labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii. The intramolecular hydrogen bond is shown as a dashed line.

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