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#### Key indicators

Single-crystal X-ray study  
 $T = 100$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.037  
 $wR$  factor = 0.099  
Data-to-parameter ratio = 7.7

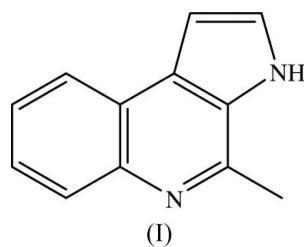
For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## 4-Methyl-3*H*-pyrrolo[2,3-*c*]quinoline

The title compound,  $\text{C}_{12}\text{H}_{10}\text{N}_2$ , is a new marine natural product which was isolated for the first time from a novel marine gliding bacterium. The asymmetric unit contains a pair of achiral molecules. Both the molecules are essentially planar and they form a dihedral angle of  $83.81(3)^\circ$ . In the crystal structure, the molecules exist as  $\text{N}-\text{H}\cdots\text{N}$  hydrogen-bonded tetramers.

### Comment

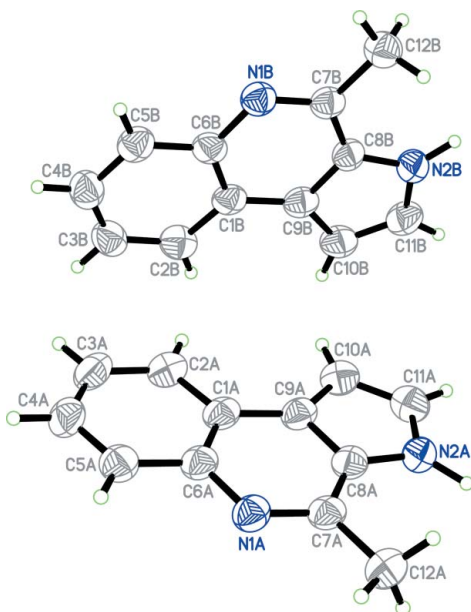
During the course of screening for biologically active substances and new secondary metabolites from marine natural products, the title compound, (I), which we named as Marinoquinoline A, was isolated for the first time from a novel marine gliding bacterium GB009, obtained from seaweed collected from Yong Ling beach, Trang province, on the southern coast of Thailand. The 16 s rRNA sequence of this gliding bacterium suggested that this gliding bacterium should be classified in a new genus because the similarity of the nucleotide sequence with the closest match (*Flexibacter aggregans*) was less than 92%. The complete identification of this bacterium is currently under investigation. The biological activity of (I) will be published elsewhere. We report here the crystal structure of (I). This is also the first report of the X-ray crystal structure of a marine natural product obtained from this bacterium.



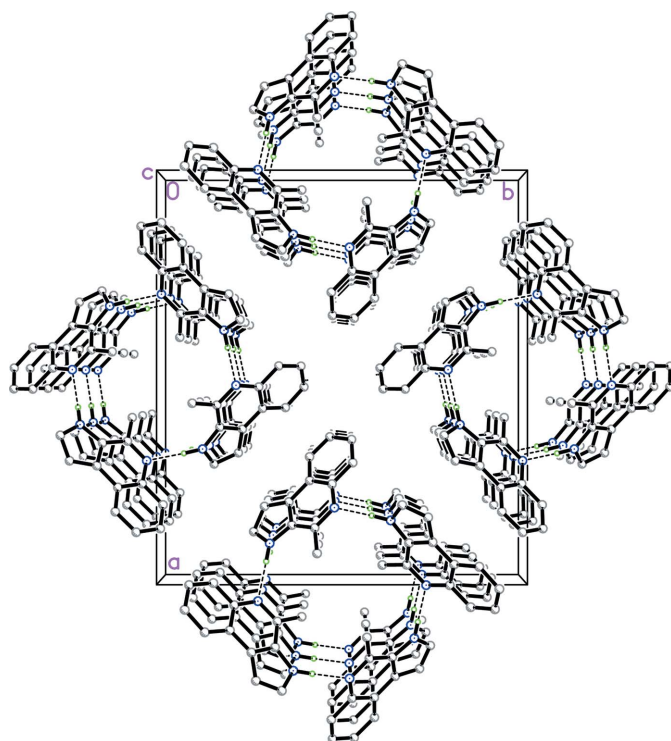
There are two molecules of (I) (*A* and *B*) in the asymmetric unit of a non-centrosymmetric space group (Fig. 1). The corresponding bond distances and angles in the two molecules agree with each other (Table 1) and show normal values (Allen *et al.*, 1987). Both the independent molecules are essentially planar with the maximum deviation of  $0.023(2)$  Å for atom N1*A* in molecule *A* and  $0.027(2)$  Å for atom C2*B* in molecule *B*. The dihedral angle between the least-squares planes of molecules *A* and *B* is  $83.81(3)^\circ$ .

In the crystal structure, pairs of molecules are linked *via* intermolecular  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds (Table 2) to form a tetramer (Fig. 2). These tetramers are stacked along the *c* axis. In addition, the molecular packing is stabilized by  $\text{C}-\text{H}\cdots\pi$  interactions.

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**Figure 1**  
The asymmetric unit of (I), showing 80% probability displacement ellipsoids and the atomic numbering.



**Figure 2**  
The crystal packing of (I), viewed down the *c* axis. Hydrogen bonds are shown as dashed lines. The C-bound H atoms have been omitted for clarity.

## Experimental

A marine gliding bacterium GB009 was cultivated in 40 flasks of 100 ml of SK liquid medium containing natural seawater and 0.2% of XAD-16 amberlite resins for 7 d. The resins were removed from the culture broth and rinsed twice with deionized water before extracting

with MeOH (4 l). The crude extract (1.07 g) obtained after evaporation of solvent was subjected to column chromatography over Sephadex LH-20 and silica gel to afford 15 mg of compound (I). Colourless needle-shaped single crystals of (I) were obtained by recrystallization from an acetone–chloroform–hexane (1:1.5:1.5) mixture after several days.

### Crystal data

$C_{12}H_{10}N_2$   
 $M_r = 182.22$   
Orthorhombic,  $P2_12_12$   
 $a = 20.2212$  (5) Å  
 $b = 18.0889$  (4) Å  
 $c = 5.1003$  (1) Å  
 $V = 1865.58$  (7) Å<sup>3</sup>

$Z = 8$   
 $D_x = 1.298$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 100.0$  (1) K  
Needle, colourless  
 $0.52 \times 0.13 \times 0.09$  mm

### Data collection

Bruker SMART APEX2 CCD area-detector diffractometer  
 $\omega$  scans  
Absorption correction: multi-scan (SADABS; Bruker, 2005)  
 $T_{\min} = 0.988$ ,  $T_{\max} = 0.993$

19204 measured reflections  
2037 independent reflections  
1847 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.038$   
 $\theta_{\max} = 25.5^\circ$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.099$   
 $S = 1.07$   
2037 reflections  
263 parameters  
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0569P)^2 + 0.4629P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.16$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.22$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

N1A—C7A	1.325 (3)	N1B—C7B	1.324 (3)
N1A—C6A	1.384 (3)	N1B—C6B	1.392 (3)
N2A—C11A	1.367 (3)	N2B—C11B	1.364 (3)
N2A—C8A	1.377 (3)	N2B—C8B	1.377 (3)
C10A—C11A	1.369 (3)	C10B—C11B	1.372 (3)
C7A—N1A—C6A	119.72 (19)	C7B—N1B—C6B	119.44 (19)
C11A—N2A—C8A	107.68 (19)	C11B—N2B—C8B	107.93 (19)
N1A—C7A—C12A	118.4 (2)	N1B—C7B—C12B	118.7 (2)
C6A—N1A—C7A—C12A	178.10 (19)	C6B—N1B—C7B—C12B	-177.90 (19)
C12A—C7A—C8A—N2A	2.5 (4)	C12B—C7B—C8B—N2B	-2.4 (4)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2A—H1NA <sup>i</sup> ⋯N1B <sup>i</sup>	0.97 (3)	1.91 (3)	2.878 (3)	178 (3)
N2B—H1NB <sup>ii</sup> ⋯N1A <sup>ii</sup>	0.93 (3)	1.95 (3)	2.875 (3)	173 (3)
C12A—H12B <sup>iii</sup> ⋯Cg1 <sup>iii</sup>	0.96	2.66	3.434 (3)	138
C12B—H12F <sup>iii</sup> ⋯Cg2 <sup>iii</sup>	0.96	2.64	3.459 (3)	143

Symmetry codes: (i)  $-x + \frac{1}{2}, y + \frac{1}{2}, -z$ ; (ii)  $x + \frac{1}{2}, -y + \frac{1}{2}, -z$ ; (iii)  $x, y, z - 1$ . Cg1 and Cg2 denote the centroids of the C8A—C11A/N2A and C8B—C11B/N2B rings, respectively.

H atoms attached to N2A and N2B were located in a difference map and isotropically refined. The remaining H atoms were placed in

calculated positions, with C—H distances of 0.93–0.96 Å. The  $U_{\text{iso}}(\text{H})$  values were constrained to be  $1.5U_{\text{eq}}$  of the carrier atom for the methyl H atoms and  $1.2U_{\text{eq}}$  for the remaining H atoms. In the absence of significant anomalous dispersion effects, 396 Friedel pairs were merged before the final refinement. The molecule is achiral.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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