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Crystal structure of 4-ethyl-3-phenylisoquinolin-1(2H)-one, $C_{17}H_{15}NO$

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.12 × 0.11 × 0.10 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.00 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	29.4°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	6380, 2244, 0.025
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1973
$N(\text{param})_{\text{refined}}$:	174
Programs:	CrysAlis ^{PRO} [1], SHELX [2], Olex2 [3]

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Abstract

$C_{17}H_{15}NO$, monoclinic, $C2/c$ (no. 15), $a = 19.197(2)$ Å, $b = 8.0719(8)$ Å, $c = 16.6511(18)$ Å, $\alpha = 90^\circ$, $\beta = 100.171(10)^\circ$, $\gamma = 90^\circ$, $V = 2539.6(5)$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.0416$, $wR_{\text{ref}}(F^2) = 0.1107$, $T = 100(1)$ K.

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The molecular structure is shown in the Figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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Source of material

Strain *Fusarium* sp. was obtained from the stem of mangrove *Sonneratia apetala* collected from Dongzhai Harbor, Hainan province, China, and identified by 18S RNA gene sequence [4]. The specimen was stored at Guangzhou Medical University, Guangzhou, P. R. China. The stored strain was recovered from solid culture medium and transferred aseptically to a 250 mL Erlenmeyer flask containing 100 mL liquid medium (glucose 10 g/L, peptone 2 g/L, yeast extract 1 g/L, sea salt 2 g/L). The fungus was cultured at 28 °C for 30 days [5]. The culture was filtered through cheesecloth. The mycelium was air-dried, extracted with methanol, and then dried with rotary evaporator. The extract was further fractionated by silica gel chromatography using a stepwise gradient solvent system according to the increasing polarity starting from 100% petroleum to 100% methanol. The title compound was isolated and purified from 75% petroleum/25% ethyl acetate fraction through silica gel column chromatography. Colorless block crystals were obtained from slow evaporation of the chloroform solution in the NMR tube at room temperature.

Experimental details

All hydrogen atoms were placed in calculated positions and refined using a riding model with the relative isotropic parameters. U_{iso} values of hydrogen atoms were set to 1.2 U_{eq} of the parent atoms.

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
O1	0.49210 (5)	0.86764 (13)	0.41927 (6)	0.0259 (3)
N1	0.42616 (6)	0.84912 (15)	0.51924 (7)	0.0209 (3)
C1	0.39462 (7)	0.52179 (18)	0.48496 (9)	0.0217 (3)
H1	0.43562	0.951238	0.531248	0.025*
C2	0.38299 (8)	0.35252 (19)	0.46581 (10)	0.0264 (4)
H2	0.359608	0.287055	0.498575	0.032*
C3	0.40561 (8)	0.28260 (19)	0.39954 (10)	0.0289 (4)
H3	0.396969	0.170945	0.388111	0.035*
C4	0.44125 (8)	0.37619 (19)	0.34927 (10)	0.0277 (4)
H4	0.454993	0.328375	0.303707	0.033*
C5	0.45585 (7)	0.53972 (19)	0.36769 (9)	0.0240 (4)
H5	0.480984	0.602027	0.335478	0.029*
C6	0.43305 (7)	0.61337 (18)	0.43489 (9)	0.0207 (3)
C7	0.45306 (7)	0.78422 (18)	0.45575 (8)	0.0207 (3)
C8	0.38463 (7)	0.76458 (18)	0.56651 (8)	0.0197 (3)
C9	0.36984 (7)	0.60136 (18)	0.55301 (9)	0.0213 (3)
C10	0.28846 (8)	0.88532 (19)	0.63265 (10)	0.0276 (4)
H10	0.255421	0.825061	0.596589	0.033*
C11	0.26581 (9)	0.9902 (2)	0.68890 (11)	0.0340 (4)
H11	0.217787	1.000215	0.690366	0.041*
C12	0.31462 (9)	1.0797 (2)	0.74261 (10)	0.0343 (4)
H12	0.299467	1.149893	0.780329	0.041*
C13	0.38618 (9)	1.06506 (19)	0.74047 (9)	0.0307 (4)
H13	0.419011	1.12509	0.776891	0.037*
C14	0.40882 (8)	0.96117 (18)	0.68415 (9)	0.0245 (4)
H14	0.456878	0.952515	0.682626	0.029*
C15	0.36025 (7)	0.86946 (17)	0.62972 (9)	0.0215 (3)
C16	0.33272 (8)	0.50005 (19)	0.60948 (10)	0.0271 (4)
H16A	0.333171	0.562445	0.65936	0.032*
H16B	0.359604	0.399318	0.623818	0.032*
C17	0.25650 (8)	0.4528 (2)	0.57485 (11)	0.0333 (4)
H17A	0.254585	0.400358	0.522754	0.050*
H17B	0.227607	0.550604	0.568467	0.050*
H17C	0.239269	0.377581	0.611505	0.050*

Comment

The title crystal structure was elucidated by MS and NMR data [6–11], and confirmed by X-ray crystallography (see the figure). The study on the biological activities of this compound has never been reported so far. Geometric parameters are all in the expected ranges [12].

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