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Crystal structure of ethyl 1-(4-fluorophenyl)-4-phenyl-1*H*-pyrrole-3-carboxylate, C₁₉H₁₆FNO₂

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.16 × 0.15 × 0.11 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.09 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	25.3°, 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	8298, 2872, 0.100
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1176
$N(\text{param})_{\text{refined}}$:	209
Programs:	Bruker [1], SHELX [2, 3]

Source of material

A 500 mL round-bottom flask was sequentially filled with 3.33 g (30 mmol) 4-fluoroaniline, 2.94 g (30 mmol) ethyl propionate, 3.96 g (30 mmol) cinnamaldehyde, 1.03 g (12 mmol) piperazine, 0.04 g (0.24 mmol) *p*-toluene-sulfonic acid and 200 mL 1,2-dichloroethane. The mixture was slowly heated to 356 K for 12 h. After the reaction, the mixture was cooled to room temperature. Two-hundred milliliters of water were slowly added, extracted with ethyl acetate for three times (100 mL/time), the organic layer was separated, washed with saturated sodium chloride solution for two times (100 mL/time), and the organic layers were combined. Dry with anhydrous sodium sulfate, filter, distill under reduced pressure to remove the solvent, and separate by silica gel column chromatography (ethyl acetate: petroleum ether = 1:50) to obtain a white powdery solid. The solid is exposed to 410 nm ultraviolet light and normal temperature light. After 24 h, the final product was obtained.

Experimental details

All hydrogen atoms were placed in the calculated positions and all the non-hydrogen atoms were refined anisotropically.

Comment

Natural products have inspired the synthesis of compounds for pharmaceutical application, most of which are

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Abstract

C₁₉H₁₆FNO₂, monoclinic, $P2_1/c$ (no. 14), $a = 10.805(7)$ Å, $b = 20.984(13)$ Å, $c = 7.034(4)$ Å, $\beta = 93.386(13)^\circ$, $V = 1592.0(17)$, $Z = 4$, $R_{\text{gt}}(F) = 0.0561$, $wR_{\text{ref}}(F^2) = 0.1336$, $T = 296$ 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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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U _{iso} */U _{eq}
F1	0.08821 (19)	0.94114 (9)	0.6579 (4)	0.1137 (9)
O1	0.3590 (2)	0.54947 (9)	0.7370 (4)	0.0748 (8)
O3	0.5604 (2)	0.53342 (11)	0.7188 (5)	0.1033 (11)
N1	0.4073 (2)	0.73707 (12)	0.6656 (4)	0.0525 (7)
C1	0.2056 (3)	0.47106 (16)	0.7586 (7)	0.1127 (16)
H1A	0.165475	0.487932	0.644082	0.169*
H1B	0.174638	0.492310	0.866947	0.169*
H1C	0.188933	0.426231	0.766606	0.169*
C2	0.3403 (3)	0.48132 (14)	0.7560 (6)	0.0916 (14)
H2A	0.381793	0.465835	0.873015	0.110*
H2B	0.373350	0.458866	0.649638	0.110*
C3	0.4750 (3)	0.56910 (15)	0.7192 (5)	0.0616 (10)
C4	0.4804 (3)	0.63826 (14)	0.6979 (5)	0.0522 (9)
C5	0.3776 (3)	0.67587 (14)	0.7041 (5)	0.0545 (9)
H5	0.299056	0.661607	0.730842	0.065*
C6	0.5317 (3)	0.73920 (15)	0.6342 (4)	0.0547 (9)
H6	0.575693	0.775670	0.605173	0.066*
C7	0.5802 (3)	0.67952 (15)	0.6524 (5)	0.0521 (9)
C8	0.7122 (3)	0.66549 (15)	0.6289 (5)	0.0552 (9)
C9	0.7787 (3)	0.62076 (15)	0.7381 (5)	0.0688 (11)
H9	0.738598	0.597624	0.828955	0.083*
C10	0.9025 (3)	0.60973 (16)	0.7153 (6)	0.0835 (13)
H10	0.944565	0.578886	0.788765	0.100*
C11	0.9642 (3)	0.64440 (19)	0.5836 (7)	0.0836 (13)
H11	1.047744	0.636971	0.567454	0.100*
C12	0.9013 (3)	0.68970 (17)	0.4774 (6)	0.0811 (13)
H12	0.942507	0.713507	0.389245	0.097*
C13	0.7773 (3)	0.70039 (15)	0.4999 (6)	0.0664 (10)
H13	0.736149	0.731695	0.427043	0.080*
C14	0.3248 (3)	0.79007 (14)	0.6631 (5)	0.0509 (9)
C15	0.3675 (3)	0.84927 (15)	0.7224 (5)	0.0640 (10)
H15	0.450186	0.854587	0.764073	0.077*
C16	0.2877 (4)	0.90032 (15)	0.7198 (5)	0.0735 (11)
H16	0.315288	0.940566	0.758146	0.088*
C17	0.1669 (4)	0.89030 (19)	0.6595 (6)	0.0738 (12)
C18	0.1225 (3)	0.83312 (18)	0.6009 (6)	0.0744 (12)
H18	0.039409	0.828208	0.561026	0.089*
C19	0.2024 (3)	0.78235 (15)	0.6012 (5)	0.0611 (10)
H19	0.173874	0.742631	0.559539	0.073*

based on *N*-heterocyclic motifs [4]. The powerful pharmaceutical and pharmacological features provided by the pyrrole nucleus as pharmacophore unit of many drugs are still recognized by medicinal chemists [5, 6]. Photochemical reactions have been widely used in various synthetic reactions [7, 8]. This time, a new pyrrole compound

was obtained by light irradiation using different reaction solvents.

In the molecules of the title crystal structure, the pyrrole ring and the aryl moieties are not in one plane. The dihedral angle of the ring formed by C14–19 and the pyrrole ring formed by N1–C7 is 59.8°. The dihedral angle between the benzene ring formed by C8–13 and the pyrrole ring formed by N1–C7 is 49.0°. The bond lengths and angles are in the expected ranges [9].

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