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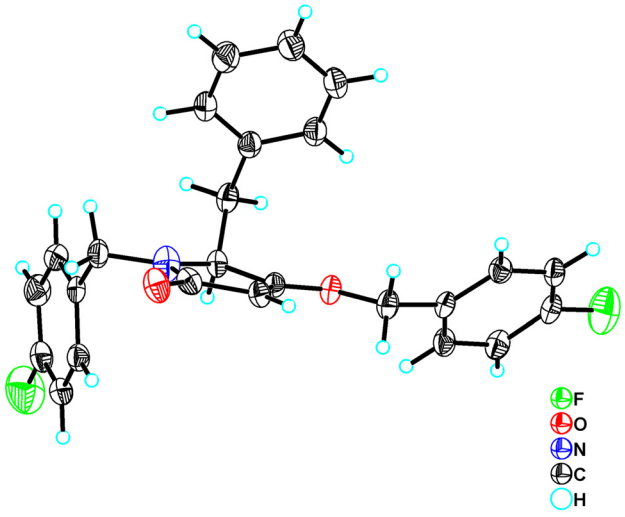
The crystal structure of 5-benzyl-1-(4-fluorobenzyl)-4-((4-fluorobenzyl)oxy)-1,5-dihydro-2*H*-pyrrol-2-one, $C_{25}H_{21}F_2NO_2$



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Abstract

$C_{25}H_{21}F_2NO_2$, triclinic, $P\bar{1}$, a = 8.2272(14) Å, b = 11.2369(12) Å, c = 13.0669(16) Å, α = 108.033(11)°, β = 107.656(13)°, γ = 100.256(12)°, V = 1044.1(3) Å^3, Z = 2, $R_{gt}(F)$ = 0.0625, $wR_{ref}(F^2)$ = 0.1820, T = 213 K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data and the list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

Table 1: Data collection and handling.

Crystal:	Light colourless block
Size:	0.14 × 0.11 × 0.09 mm
Wavelength:	Cu *Kα* radiation (1.54184 Å)
μ:	0.77 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω scans
θ_{max}, completeness:	75.4°, 99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6543, 4063, 0.035
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3,036
N(param)$_{refined}$:	271
Programs:	Rigaku[1], Shelx[2], Olex2[3]

1 Source of materials

To a solution fo 5-benzylpyrrolidine-2,4-dione (189 mg, 1 mmol) in MeCN (10 mL) was added 1-(bromomethyl)-4-fluorobenzene (473 mg, 2.5 mmol) and K_2CO_3 (415 mg, 3 mmol), and the resulting mixture was stirred under reflux for 2 h. After completion of the reaction, the reaction mixture was cooled to room temperature, water (50 mL) was added and extracted with ethyl acetate (20 mL). The organic layer was dried with anhydrous Na_2SO_4, and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel to afford compound 5-benzyl-1-(4-fluorobenzyl)-4-((4-fluorobenzyl)oxy)-1,5-dihydro-2*H*-pyrrol-2-one (296 mg, 73 % yield) as a white solid.

2 Experimental details

The Shelxl[2] refinement package was employed to refine the crystal structure. The Olex2[3] was used to visualize the crystal structure. All hydrogen atoms were placed in idealized positions. Their U_{iso} values were set to 1.2U_{eq} of the parent atoms.

3 Comment

1,5-Dihydro-2*H*-pyrrol-2-one represents a class of significant five-membered nitrogen-containing heterocycles. Their structural motifs are ubiquitously present in diverse natural molecules and synthetic compounds, exhibiting broad-

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Xin-Yan Shao, Pan-Pan Wu and Ming Lang, School of Pharmacy and Food Engineering, Wuyi University, Jiangmen, Guangdong, 529020, P.R. China. https://orcid.org/0009-0002-5374-0427 (P.-P. Wu)

spectrum biological activities. Within this chemical family, numerous substances with antibacterial, anti-inflammatory, and antitumor activities have been identified,[4,5] such as jatropham[6] and 4,5-dimethyl-3-ethyl-5-hydroxy-3-pyrrolin-2-one.[7] Notably, *N*-(5-tert-butyl-1,3,4-thiadiazol-2-yl)-3,4-dimethyl-5-oxo-3-pyrrolin-2-ones demonstrate remarkable herbicidal efficacy at low dosages while maintaining no adverse effects on normal plant growth.[8–10] The study employed crystallographic analysis to investigate both the spatial arrangement of molecules and their intermolecular bonding patterns. The bond distance of F1–C23 and F2–C16 is 1.366(4) and 1.365(3) Å. The bond lengths of O1–C1, O2–C3 and O2–C12 are 1.218(4), 1.338(3) and 1.452(3) Å. The C1–N1–C19, and C4–N1–C19 angles are 123.7(2) and 123.2(2)°, respectively, while those for C1–N1–C4 is 112.8(2)°. All of the hydrogen atoms were placed in the calculated positions. The bond lengths and angles within the molecule are within the expected ranges.[9,10]

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Conflict of interest: The authors declare no conflicts of interest regarding this article.

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