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The crystal structure of topiroxostat, $C_{13}H_8N_6$

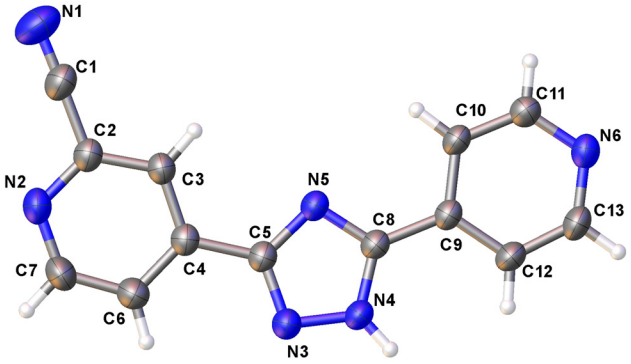

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.15 × 0.10 × 0.10 mm
Wavelength:	CuKα radiation (1.54184 Å)
μ:	0.77 mm^{-1}
Diffractometer, scan mode:	Rigaku Synergy, ω scans
θ_{max}, completeness:	76.3°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	11157, 2312, 0.019
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2,121
$N(param)_{refined}$:	176
Programs:	Rigaku,[1] Olex2,[2] SHELX[3,4]

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Abstract

$C_{13}H_8N_6$, monoclinic, $P2_1/c$ (no. 14), a = 7.34720(10) Å, b = 12.9562(3) Å, c = 12.1399(2) Å, β = 97.071(2)°, V = 1146.83(4) Å^3, Z = 4, $R_{gt}(F)$ = 0.0438, w$R_{ref}(F^2)$ = 0.1169, T = 297 K.

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

1 Source of materials

The title compound (topiroxostat, systematic name: 4-(5-(pyridin-4-yl)-1*H*-1,2,4-triazol-3-yl)picolinonitrile) was bought from Shanghai Titan Technology Co. Ltd. About 1 g topiroxostat powder was placed into a 10 ml penicillin bottle, followed by addition of 5 ml N-methyl pyrrolidone. After the suspension solution was thoroughly mixed, the bottle was sealed with a cap and placed in an oven. The bottle was maintained at a temperature of 400 K until all the powder was completely dissolved. The vial was then removed from the oven and left at room temperature. After one week, block crystals were harvested.

2 Experimental details

The positions of hydrogen atoms on carbon atoms were calculated geometrically and refined using the riding model. Their displacement parameters were constrained to ride on the carrier atom. The hydrogen atom on the nitrogen atom was located from difference Fourier map. The distance between the hydrogen atom and the nitrogen atom was refined freely. A DFIX restrain was used to get a better model for the hydrogen atom.

3 Comment

Topiroxostat is a non-purine selective xanthine oxidase inhibitor.[5] It works by inhibiting the activity of xanthine oxidase, thereby reducing the production of uric acid and consequently lowering the levels of uric acid in the blood.[6] Topiroxostat exhibits high selectivity and potency, and compared to other xanthine oxidase inhibitors, it demonstrates favorable safety and tolerability in clinical applications.[7]

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The titled compound was crystallized in $P2_1/c$ space group with one molecule in its asymmetric unit. The bond lengths and angles within these moieties are in the expected ranges. The molecular structure comprises two pyridine rings and one central imidazole ring. The torsion angle of N4–C8–C9–C12 is 2.53(19)°, while the torsion angle of C6–C4–C5–N3 is −9.11(18)°. These torsion angles indicate that the three rings are not entirely coplanar but instead form a certain angle with each other. An intermolecular hydrogen bond is formed between N4 atom on the imidazole ring and $N6^{-x,1/2+y,1/2-z}$ atom on the pyridine ring, with a bond length of 2.8350(14) Å.

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

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