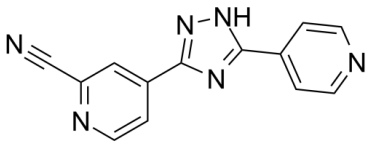
Data Sheet

Product Name:	Topiroxostat
Cat. No.:	CS-2033
CAS No.:	577778-58-6
Molecular Formula:	C13H8N6
Molecular Weight:	248.24
Target:	Cytochrome P450; Xanthine Oxidase
Pathway:	Metabolic Enzyme/Protease
Solubility:	DMSO : 23.5 mg/mL (94.67 mM; Need ultrasonic and warming)



BIOLOGICAL ACTIVITY:

Topiroxostat (FYX-051) is a potent and orally active **xanthine oxidoreductase (XOR)** inhibitor with an **IC_{50}** value of 5.3 nM and a **K_i** value of 5.7 nM. Topiroxostat exhibits weak **CYP3A4**-inhibitory activity (18.6%). Topiroxostat has the potential for hyperuricemia treatment[1][2]. IC50 & Target: IC50: 5.3 nM (XOR)[1]

Ki: 5.7 nM (XOR)[2] **In Vitro:** These potent and more sustained effects of Topiroxostat (FYX-051, compound 39) have been confirmed by a crystallographic analysis of XOR-Topiroxostat complex. The cyano group of Topiroxostat has been reported to play an important role in the binding activity between Topiroxostat and XOR. This is attributable to the formation of a hydrogen bond between Asn 768 of XOR and the cyano group of Topiroxostat[1]. **In Vivo:** Topiroxostat (FYX-051; 0.03-10 mg/kg; oral administration; for 1 hour; male Wistar/ST strain rats) treatment shows a potent and long-lasting hypouricemic effect in a rat model of potassium oxonate-induced hyperuricemia[2] .

The C_{max} and bioavailability of Topiroxostat (FYX-051, compound 39) are as high as 4.62 μg/mL (3 mg/kg) and 69.6%, respectively. Moreover, the $t_{1/2}$ value of Topiroxostat is 19.7 hours[1].

References:

[1]. Sato T, et al. Discovery of 3-(2-cyano-4-pyridyl)-5-(4-pyridyl)-1,2,4-triazole, FYX-051 - a xanthine oxidoreductase inhibitor for the treatment of hyperuricemia [corrected]. Bioorg Med Chem Lett. 2009 Nov 1;19(21):6225-9.

[2]. Matsumoto K, et al. FYX-051: a novel and potent hybrid-type inhibitor of xanthine oxidoreductase. J Pharmacol Exp Ther. 2011 Jan;336(1):95-103.

CAIndexNames:

2-Pyridinecarbonitrile, 4-[3-(4-pyridinyl)-1H-1,2,4-triazol-5-yl]-

SMILES:

N#CC1=NC=CC(C2=NNC(C3=CC=NC=C3)=N2)=C1

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