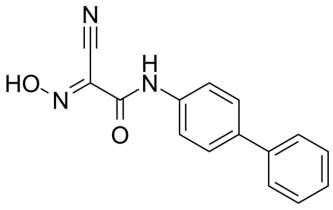
DHODH-IN-11

Cat. No.:	HY-135675
CAS No.:	1263303-95-2
Molecular Formula:	$C_{15}H_{11}N_3O_2$
Molecular Weight:	265.27
Target:	Dihydroorotate Dehydrogenase; DNA/RNA Synthesis
Pathway:	Metabolic Enzyme/Protease; Cell Cycle/DNA Damage
Storage:	-20°C, protect from light * In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 125 mg/mL (471.22 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.7697 mL	18.8487 mL	37.6974 mL
	5 mM	0.7539 mL	3.7697 mL	7.5395 mL
	10 mM	0.3770 mL	1.8849 mL	3.7697 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: 2.08 mg/mL (7.84 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

DHODH-IN-11 (Compound 14b) is a Leflunomide derivative and a weak dihydroorotate dehydrogenase (DHODH) inhibitor with a pK_a of 5.03[1].

IC_{50} & Target

pKa: 5.03 (DHODH)[1]

In Vitro

Designed a compound structurally related to Leflunomide, containing the furazan ring (Compound 14a), is designed. Compound 14a undergo ring 4 scission under physiological pH conditions to afford the corresponding cyano-oximes DHODH-IN-11 (Compound 14b). DHODH-IN-14 has been assayed as a DHODH inhibitor; its low potency is probably due to the unfavourable stereochemistry of the oxime substructure[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Giorgis M, et al. 1,2,5-Oxadiazole analogues of leflunomide and related compounds. Eur J Med Chem. 2011 Jan;46(1):383-92.

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