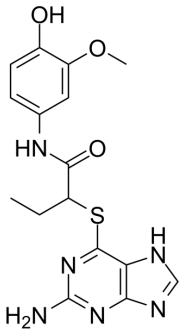
Enpp-1-IN-12

Cat. No.:	HY-143256
CAS No.:	2631703-41-6
Molecular Formula:	$C_{16}H_{18}N_6O_3S$
Molecular Weight:	374.42
Target:	Phosphodiesterase (PDE)
Pathway:	Metabolic Enzyme/Protease
Storage:	4°C, sealed storage, away from moisture and light * In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture and light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (133.54 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.6708 mL	13.3540 mL	26.7080 mL
	5 mM	0.5342 mL	2.6708 mL	5.3416 mL
	10 mM	0.2671 mL	1.3354 mL	2.6708 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: ≥ 1 mg/mL (2.67 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1 mg/mL (2.67 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Enpp-1-IN-12 (compound 43) is a potent and orally active ecto-nucleotide pyrophosphatase/phosphodiesterases 1 (ENPP1) inhibitor, with a Ki of 41 nM. Enpp-1-IN-12 exhibits anti-tumor activity[1].

IC_{50} & Target

Ki: 41 nM (ENPP1)[1]

In Vitro

Enpp-1-IN-12 (5 μM) exhibits half-life and intrinsic clearance of >120 min and <11.55 μL/min/million cells and 61.88 min and 22.4 μL/min/million cells in human and mouse hepatocytes, respectively[1].

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

In Vivo

Enpp-1-IN-12 (100 mg/kg; p.o.) inhibits tumor growth in LLC1 syngeneic murine tumor model for lung cancer[1].

Enpp-1-IN-12 (10 mg/kg; p.o.) exhibits moderate oral bioavailability (F=45.1%), half-life ($t_{1/2}$=1.04 h), and C_{max} (303.10

	ng/mL) in healthy female BALB/c mice[1]. Enpp-1-IN-12 (1 mg/kg; i.v.) exhibits half-life ($t_{1/2}$=0.76 h), C_{max} (308.64 ng/mL), and CL of 73.22 mL/min/kg in healthy female BALB/c mice[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Gangar M, et, al. Design, synthesis and biological evaluation studies of novel small molecule ENPP1 inhibitors for cancer immunotherapy. Bioorg Chem. 2022 Feb;119:105549.

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