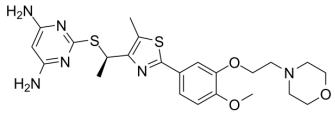
DI-87

Cat. No.:	HY-133141
CAS No.:	2107280-55-5
Molecular Formula:	$C_{23}H_{30}N_6O_3S_2$
Molecular Weight:	502.65
Target:	Others
Pathway:	Others

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 145 mg/mL (288.47 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.9895 mL	9.9473 mL	19.8946 mL
5 mM	0.3979 mL	1.9895 mL	3.9789 mL
10 mM	0.1989 mL	0.9947 mL	1.9895 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: ≥ 2.5 mg/mL (4.97 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (4.97 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (4.97 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

DI-87 is an orally active and selective deoxycytidine kinase (dCK) inhibitor with an EC_{50} of 10.2 nM. DI-87 has antitumor activity and is used in combination therapy against tumors expressing dCK[1].

IC_{50} & Target

EC50: 10.2 nM (dCK)[1]

In Vitro

(S)-DI-87 exhibits a much higher IC_{50} value (IC_{50}=468 nM) relative to DI-87 ((R)-DI-8) (IC_{50}=3.15 nM) in CEM T-ALL cells for inhibition of dCK activity[1].

DI-87 (1 μM; for 72 hours) rescues human cell line CCRF-CEM (CEM) cells from the anti-proliferative effects of gemcitabine, a dCK-dependent nucleoside analog prodrug, with an EC_{50} of 10.2 nM[1].

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

In Vivo

DI-87 (5-25 mg/kg; oral gavage) exhibits full dCK inhibition for 27 hours, and enzyme activity fully recovered by 36 hours with 25 mg/kg dose[1].

DI-87 (10-50 mg/kg; oral) has plasma concentrations of between 1 and 3 hours and plasma half-life of 4 hours[1].

DI-87 (10 mg/kg/day or 25 mg/kg/twice a day; oral; for 16-18 days) with thymidine (2 g/kg; ip; twice a day) results in reduced tumor growth in male NSG mice implanted with CEM tumors[1].

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

Animal Model:	8-12 week-old male or female NSG mice with CEM tumor xenografts[1]
Dosage:	5, 10, 25 mg/kg
Administration:	Oral gavage
Result:	The 25 mg/kg dose exhibited full dCK inhibition for 27 hours, and enzyme activity fully recovered by 36 hours. The 10 mg/kg dose resulted in full inhibition with recovery initiating at the 12 hours time point. The 5 mg/kg dose resulted in minimal dCK inhibition with rapid recovery.

Animal Model:	Female NSG mice with CEM tumors[1]
Dosage:	10, 25, or 50 mg/kg
Administration:	Oral
Result:	Had plasma concentrations of between 1 and 3 hours and plasma half-life of 4 hours. Had tumor concentrations lower than plasma and had a later, more sustained peak at 3-9 hours.

REFERENCES

[1]. Soumya Poddar, et al. Development and Preclinical Pharmacology of a Novel dCK Inhibitor, DI-87. Biochem Pharmacol. 2020 Feb;172:113742.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA