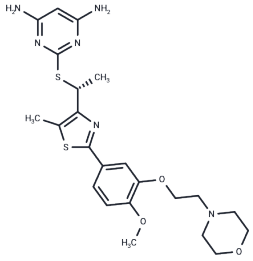
Data Sheet (Cat.No.T39550)

TargetMol

DI-87

Chemical Properties



CAS No. : 2107280-55-5

Formula: C23H30N6O3S2

Molecular Weight: 502.65

Storage: Store at low temperature
Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	DI-87 (TRE-515) is a novel and orally available dCK (deoxycytidine kinase) inhibitor with good in vitro activity and low protein binding. DI-87 binds to dCK and prevents the phosphorylation of deoxycytidine by dCK, which reduces the production of dNTP and cell cycle arrest (especially in S phase). When combined with thymidine, DI-87 significantly inhibits tumor growth.
Targets(IC50)	Others,DNA/RNA Synthesis
In vitro	**Methods**: CEM cells were seeded at 1 × 10 3 cells/well in white opaque 384-well plates at 50 μl/well and treated as indicated. After incubation with increasing concentrations (2 nM-10 μM) of gemcitabine and 1 μM DI-87 for 72 h, 50 μl of CellTiter-Glo reagent (diluted 1:5 in dH2O) was added to each well, the plates were incubated at room temperature for 5 m, and luminescence was measured using a BioTek microplate luminometer. **Results**: The cytotoxic effect of gemcitabine requires dCK, and administration of DI-87 completely blocked cytotoxicity after gemcitabine treatment, demonstrating dCK inhibition by DI-87. [1]
In vivo	**Methods**: Female NSG mice bearing CEM tumors were treated with DI-87 (10, 25, or 50 mg/kg, orally) and DI-87 plasma and tumor concentrations were assessed. **Results**: Plasma DI-87 concentrations peaked between 1 and 3 hours; tumor concentrations were lower than plasma and had a later, more sustained peak at 3-9 hours. [1]

Solubility Information

Solubility	DMSO: 120 mg/mL (238.73 mM),Sonication and heating are recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 4 mg/mL (7.96 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
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
50 mM	0.0398 mL	0.1989 mL	0.3979 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

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