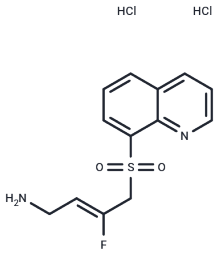
Data Sheet (Cat.No.T39986)

TargetMol

LOX-IN-3 dihydrochloride

Chemical Properties



CAS No. : 2409964-23-2

Formula: C13H15Cl2FN2O2S

Molecular Weight: 353.24

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	LOX-IN-3 dihydrochloride, an inhibitor of lysyl oxidase (LOX), inhibits bovine LOX (IC50<10 μM) and human LOXL2 (IC50<1 μM) activities.
Targets(IC50)	Lipoxygenase,Monoamine Oxidase
In vitro	LOX-IN-3 (Compound 33) inhibits the bovine LOX and human LOXL2 activities with IC 50 values of <10 μM and <1 μM, respectively. LOX-IN-3 is less active against SSAO/VAP-1 and MAO-B activities[1].
In vivo	In young male Wistar rats, a single high (30 mg/kg) dose of LOX-IN-3 (Compound 33) completely abolishes lysyl oxidase activity. While plasma concentrations of LOX-IN-3 are far below the IC50 after 8 hours, the half-life of recovery is between 2-3 days (ear) and 24 hours (aorta)[1]. In a 14-day unilateral ureteric obstruction (UUO) model, LOX-IN-3 (Compound 33, 10 mg/kg daily; orally) treatment increases kidney weight and thickness and reduces the area of fibrosis as measured by Picrosirius Red[1]. In BALB/c mice bearing hepatic fibrosis, LOX-IN-3 (Compound 33, 20 mg/kg daily, i.p.) treatment significantly reduces liver fibrosis. At the end of week 4 a mouse breast cancer cell line (4tl) is injected orthotopically. LOX-IN-3 (Compound 33) treatment significantly reduces liver fibrosis, collagen cross-links and the metastatic load in the liver[1].

Solubility Information

Solubility	DMSO: 55 mg/mL (155.7 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (5.66 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	2.8309 mL	14.1547 mL	28.3094 mL
5 mM	0.5662 mL	2.8309 mL	5.6619 mL
10 mM	0.2831 mL	1.4155 mL	2.8309 mL
50 mM	0.0566 mL	0.2831 mL	0.5662 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

Alison Dorothy Findlay, et al. Haloallylamine sulfone derivative inhibitors of lysyl oxidases and uses thereof. WO2020024017A1.