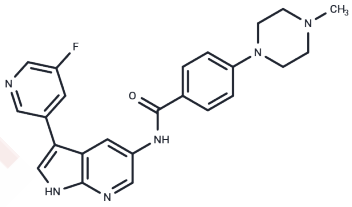
Data Sheet (Cat.No.T72039)

TargetMol

CLK1-IN-3

Chemical Properties



CAS No. : 2922550-28-3

Formula: C24H23FN6O

Molecular Weight: 430.48

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	Clk1-in-3 is a + selective and highly potent sexual Clk1 inhibitor with an IC50 of 5 nM and 300 pairs higher affinity than Dyrk1A. CLK1-IN-3 also showed highly effective inhibition of Clk2 and Clk4, with IC50 values of 42 and 108 nM, respectively. CLK1-IN-3 is effective in inducing autophagy in vitro and can be used for prevention and human treatment of acute liver injury (ALI).
Targets(IC50)	CDK,Autophagy,DYRK
In vitro	CLK1-IN-3 (compound 10ad) demonstrates anti-tumor potential through dual inhibition of Clk1 and Clk2. At concentrations ranging from 10 μM to 1000 μM, it effectively binds to Clk1 protein and inhibits its degradation dose-dependently. Additionally, CLK1-IN-3 (0-10 μM, 24 h) induces autophagy in Hela, BNLCL.2, and HCT 116 cells and stimulates the degradation of SQSTM1/p62 (autophagy marker)[1].
In vivo	CLK1-IN-3 (0-40 mg/kg, intraperitoneal injection, single dose) significantly inhibits acute liver injury induced by acetaminophen (APAP) in the ALI model, and there is no apparent hepatocyte death observed[1]. CLK1-IN-3 (10 mg/kg; intravenous injection, oral administration, intraperitoneal injection, single dose) exhibits acceptable pharmacokinetic characteristics, with a relatively long half-life (T1/2) of 5.29 hours and an oral bioavailability of 19.5%[1].

Solubility Information

Solubility	DMSO: 55 mg/mL (127.76 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 (4.65 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	2.323 mL	11.6149 mL	23.2299 mL
5 mM	0.4646 mL	2.323 mL	4.646 mL
10 mM	0.2323 mL	1.1615 mL	2.323 mL
50 mM	0.0465 mL	0.2323 mL	0.4646 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

Yang T, et al. Rational design and appraisal of selective Cdc2-Like kinase 1 (Clk1) inhibitors as novel autophagy inducers for the treatment of acute liver injury (ALI). Eur J Med Chem. 2023 Mar 15;250:115168.