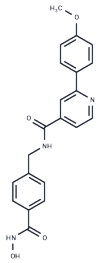
Data Sheet (Cat.No.T77334)

TargetMol

HDAC-IN-57

Chemical Properties



CAS No. : 2716217-79-5

Formula: C21H19N3O4

Molecular Weight: 377.39

Storage: 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	HDAC-IN-57 is an orally active pan-inhibitor of histone deacetylase (HDAC), inhibiting HDAC1, HDAC2, HDAC6, and HDAC8 with IC50 values of 2.07 nM, 4.71 nM, 2.4 nM, and 107 nM, respectively. HDAC-IN-57 inhibits LSD1 with an IC50 value of 1.34 μM. HDAC-IN-57 has anti-tumor activity and can induce apoptosis.
Targets(IC50)	Apoptosis,HDAC
In vitro	HDAC-IN-57 (Compound 5e) (1.0 μM, 2.5 μM, 5.0 μM; 48 h) effectively suppresses the migration and invasion of solid tumor cell lines, namely MGC-803, A549, and HCT-116. Furthermore, HDAC-IN-57 demonstrates significant growth inhibition in these solid tumor cell lines, exhibiting IC50 values of 0.45 μM, 1.48 μM, and 0.57 μM, respectively. Additionally, HDAC-IN-57 elicits apoptosis in MGC-803 and HCT-116 cells in a dose-dependent manner. It also exerts inhibitory effects on LSD1 and HDACs within the MGC-803 and HCT-116 cell lines. Moreover, HDAC-IN-57 induces cell cycle arrest in the G2/M phase for both MGC-803 and HCT-116 cells.[1] HDAC-IN-57 has high metabolic stability in vitro. Retains 86.1% and 87.4% of the parent compound after 1 hour of incubation in human liver (HLM) and rat liver microsomes (RLM), respectively, with a T1/2 of over 120 minutes.[1]
In vivo	HDAC-IN-57 (Compound 5e) (1 mg/kg, i.v.; 10 mg/kg, p.o.) demonstrated T1/2 of 0.37 hours (IV) and 2.75 hours (OR), with an oral bioavailability (F%) of 10.6%.[1] HDAC-IN-57 (25 or 50 mg/kg gavage; once daily for 21 days) achieved dose-dependent tumor growth inhibition in the NOD-SCID mouse MGC-803 xenograft model.[1]

Solubility Information

Solubility	DMSO: 250 mg/mL (662.44 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.6498 mL	13.2489 mL	26.4978 mL
5 mM	0.530 mL	2.6498 mL	5.2996 mL
10 mM	0.265 mL	1.3249 mL	2.6498 mL
50 mM	0.053 mL	0.265 mL	0.530 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

Duan, Yingchao, et al. Preparation of 2-arylisonicotinamide derivatives as LSD1/HDAC dual target inhibitors for treatment of acute myeloid leukemia. CN113444038