Data Sheet (Cat.No.T74783)

TargetMol

HDAC-IN-53

Chemical Properties

CAS No. : 2921948-27-6

Formula: C23H20ClN7O2

Molecular Weight: 461.9

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-53 is an orally active, selective inhibitor of HDAC1-3, with IC50 values of 47 nM, 125 nM, and 450 nM, respectively. It exhibits no inhibitory effects on class II HDACs (HDAC4, 5, 6, 7, 9; IC50 >10 μM). The compound induces caspase-dependent apoptosis and significantly hampers the growth of human tumor xenografts in nude mice and murine tumor growth in immune-competent mice with MC38 colon cancer [1].
Targets(IC50)	Apoptosis,HDAC
In vitro	HDAC-IN-53 (Compound 19h) exhibits robust antiproliferative activity against a panel of cancer cell lines, such as MC38 (IC50 = 0.66 μM) and HCT116 cells (IC50 = 0.56 μM) [1]. At concentrations ranging from 0.1 to 1 μM over 24 hours, HDAC-IN-53 induces G0/G1 cell cycle arrest in MC38 cells and G2/M cell cycle arrest in HCT116 cells [1]. Additionally, the same treatment with HDAC-IN-53 dose-dependently upregulates the expression of cleaved caspase-3 and cleaved PARP [1].
In vivo	HDAC-IN-53, administered orally at doses of 60 or 120 mg/kg once daily for 15 days, exhibited antitumor activity through both direct inhibition of tumor growth and indirect immune cell-mediated antitumor effects[1]. The pharmacokinetic parameters of HDAC-IN-53 in mice are reported as follows[1]: after intravenous (IV) administration at 5 mg/kg, the time to maximum concentration (Tmax) is 0.42 hours, with a maximum concentration (Cmax) of 8129 ng/mL. The area under the curve (AUC0-t) is 5864 ng/mLh, and the half-life (t1/2) is 0.85 hours. In contrast, after oral administration (PO) at 20 mg/kg, Tmax is 0.42 hours, Cmax is 9558 ng/mL, AUC0-t is 15278 ng/mLh, t1/2 is 2.49 hours, and the bioavailability (F%) is 65.1%.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.165 mL	10.8249 mL	21.6497 mL
5 mM	0.433 mL	2.165 mL	4.3299 mL
10 mM	0.2165 mL	1.0825 mL	2.165 mL
50 mM	0.0433 mL	0.2165 mL	0.433 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.