Data Sheet (Cat.No.T61433)

TargetMol

HDAC1-IN-5

Chemical Properties

CAS No. :

Formula: C20H21N3O2S

Molecular Weight: 367.46

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	HDAC1-IN-5, a potent inhibitor of HDAC1 with an IC50 value of 15 nM, also exhibits inhibitory activity towards HDAC6 with an IC50 value of 20 nM. In cancer cells, HDAC1-IN-5 enhances the acetylation of both histone H3 and α-tubulin, leading to the activation of caspase 3 and induction of apoptosis. Additionally, HDAC1-IN-5 binds with DNA, causing chromatin damage. Furthermore, it demonstrated strong inhibitory activity against tumor growth in xenograft mice. [1]
Targets(IC50)	Apoptosis,Others,Caspase,Microtubule Associated,HDAC
In vitro	HDAC1-IN-5 (compound 4j), across a range of concentrations (0-50 μM; 48 h), demonstrates potent inhibitory effects on several cell lines, including HCT116, HeLa, HepG2, MC38, K562, and HEL, exhibiting IC50 values of 0.47 μM, 0.78 μM, 1.4 μM, 0.43 μM, 0.91 μM, and 0.28 μM, respectively [1]. At lower concentrations (0.16-1.5 μM; 48 h), HDAC1-IN-5 triggers apoptosis in HCT116 cells in a dose-dependent manner, inducing 38.5% apoptosis at 1.5 μM [1]. Additionally, HDAC1-IN-5 (0.17-1.5 μM; 24 h or 48 h) leads to the downregulation of SPT16 and SSRP-1, caspase-3 cleavage, and an increase in Acetyl-Histone H3 and Acetyl-α-tubulin expression in HCT116 and MC38 cells, demonstrating a mechanism involving modulation of both cell proliferation and apoptotic pathways in a dose-dependent fashion [1].
In vivo	HDAC1-IN-5 administered intraperitoneally (IP) at dosages of 50 and 100 mg/kg every two days for 16 days significantly reduced tumor volume and weight in MC38 xenograft mice models composed of C57BL/6 mice aged 6-10 weeks, into which 2×10^6 MC38 cells were subcutaneously injected into the right flank regions. This therapy achieved a tumor growth inhibition (TGI) rate of 66% at the 50 mg/kg dosage.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.7214 mL	13.6069 mL	27.2138 mL
5 mM	0.5443 mL	2.7214 mL	5.4428 mL
10 mM	0.2721 mL	1.3607 mL	2.7214 mL
50 mM	0.0544 mL	0.2721 mL	0.5443 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.