Data Sheet (Cat.No.T201795)

TargetMol

HDACs/EZH2-IN-1

Chemical Properties

CAS No. :

Formula: C29H36BrN7O4

Molecular Weight: 626.54

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	HDACs/EZH2-IN-1 (Compound 22a) is a dual inhibitor of HDACs and EZH2, exhibiting potent inhibitory activity, with EZH2 Y641N being suppressed by 98% at 50 nM. It selectively targets HDAC1 and HDAC6, with IC50 values of 0.23 μM and 0.07 μM, respectively. HDACs/EZH2-IN-1 effectively inhibits the proliferation of diffuse large B-cell lymphoma cells harboring EZH2 mutations and various acute myeloid leukemia cells. Additionally, this compound has the capability to induce cellular differentiation and apoptosis (Apoptosis).
Targets(IC50)	Histone Methyltransferase,Endogenous Metabolite,HDAC
In vitro	HDACs/EZH2-IN-1 demonstrates significant antiproliferative effects on SU-DHL-6 DLBCL cells carrying the EZH2 Y641N mutation, achieving IC50 values of 1.04 μM at 48 h and 0.17 μM at 120 h (5 μM, 48-120 h). Additionally, this compound inhibits the growth of AML cells with IC50 values of 1.39 μM (MV4-11), 2.45 μM (U937), and 1.32 μM (OCI-AML3) at concentrations ranging from 0.1 to 100 μM over 48 hours. It also elevates intracellular levels of HDAC1/2/3 substrate acetyl-histone H3 (AC-HH3) and HDAC6 substrate acetyl-α-tubulin (AC-α-tubulin) within the same dosage and timeframe. At 2 μM for 48 hours, HDACs/EZH2-IN-1 induces differentiation in MOLM13 cells, reflected by increased expression of the myeloid maturation markers CD11b and CD14 and provokes dose-dependent apoptosis at 2-4 μM. When used in conjunction with anti-AML agents (cytarabine, doxorubicin, and gilteritinib), HDACs/EZH2-IN-1 potentiates anticancer effects on MOLM13 cells at doses of 1-2 μM. Moreover, the compound exhibits good metabolic stability in human and rat plasma, with half-lives exceeding 180 minutes and 138 minutes, respectively.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.5961 mL	7.9803 mL	15.9607 mL
5 mM	0.3192 mL	1.5961 mL	3.1921 mL
10 mM	0.1596 mL	0.798 mL	1.5961 mL
50 mM	0.0319 mL	0.1596 mL	0.3192 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.