Data Sheet (Cat.No.T61474)

TargetMol

HDAC6-IN-13

Chemical Properties

CAS No. :

Formula: C23H22N4O

Molecular Weight: 370.45

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	HDAC6-IN-13 (Compound 35m) is a potent and highly selective orally active inhibitor of HDAC6, with an IC50 of 0.019 μM. It also inhibits HDAC1, HDAC2, and HDAC3, with IC50 values of 1.53 μM, 2.06 μM, and 1.03 μM, respectively. HDAC6-IN-13 exhibits substantial blood-brain barrier permeability and anti-inflammatory properties [1].
Targets(IC50)	Others,HDAC
In vitro	HDAC6-IN-13 (Compound 35m), at concentrations ranging from 0.1 to 1 μM over 24 hours, demonstrates high selectivity for HDAC6 over class I HDAC enzymes. This compound is characterized by its slow-on and slow-off tight-binding inhibition of HDAC6, contrasting with its rapid binding affinity for HDAC1, 2, and 3. Furthermore, HDAC6-IN-13 exhibits anti-inflammatory effects in vitro at higher concentrations of 5 to 20 μM after an 8-hour exposure. Western Blot Analysis on the MV4 11 and J774A.1 cell lines, using 0.1, 0.2, 0.5, and 1 μM concentrations for 24 hours, revealed a concentration-dependent increase in acetylated tubulin (Ac-Tubulin), with no significant changes in acetylated histone H3 (AcHH3) and H4 (AcHH4) at the 1 μM level. Another analysis on J774A.1 cells, at concentrations of 5, 10, and 20 μM for 8 hours, demonstrated dose-dependent inhibition of pro-caspase 1 cleavage to p20 and prevented the interaction between HDAC6 and dynein, highlighting its potential for therapeutic applications in inflammation and cancer.
In vivo	HDAC6-IN-13 (Compound 35m), administered at 20 mg/kg both orally (p.o.) and intraperitoneally (i.p.), significantly reduces LPS-induced inflammation in mice, demonstrating potent anti-inflammatory effects. When administered orally at the same dosage, it exhibits high bioavailability (93.4%) and substantial blood-brain barrier (BBB) permeability. Tested in male C57BL/6 WT mice using an LPS-induced endotoxic shock model and male CD-1 mice for pharmacokinetic studies, HDAC6-IN-13 significantly decreased serum IL-1β levels. Pharmacokinetic analysis revealed a maximum plasma concentration (Cmax) of 4604 ± 551 ng/mL (i.v., 5 mg/kg) and 5570 ± 551 ng/mL (p.o., 20 mg/kg), half-life (t1/2) of 7.95 ± 0.370 h (i.v.) and 6.80 ± 0.145 h (p.o.), and area under the curve (AUC) of 2755 ± 395 ng·h/mL (i.v.) and 10292 ± 1385 ng·h/mL (p.o.). Blood samples analyzed via LC-MS/MS confirm the compound's effective delivery and promising pharmacodynamic profile for combatting inflammation.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.6994 mL	13.4971 mL	26.9942 mL
5 mM	0.5399 mL	2.6994 mL	5.3988 mL
10 mM	0.2699 mL	1.3497 mL	2.6994 mL
50 mM	0.054 mL	0.2699 mL	0.5399 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.