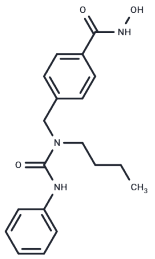
Data Sheet (Cat.No.T1819)

TargetMol

Nexturastat A

Chemical Properties



CAS No. : 1403783-31-2

Formula: C19H23N3O3

Molecular Weight: 341.4

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	Nexturastat A is an effective and specific HDAC6 inhibitor (IC50: 5 nM). Its selectivity is >190-fold than other HDACs.
Targets(IC50)	HDAC
In vivo	Nexturastat A significantly inhibits the growth of B16 melanoma cells in mice, with a GI50 of 14.3 μM. In these cells, Nexturastat A dose-dependently increases the levels of acetylated α-tubulin without affecting the acetylation of histone H3 associated with abscesses.
Kinase Assay	HDAC inhibition assays: HDAC inhibition assays are performed by Reaction Biology Corp. using isolated human, recombinant full2length HDAC1 and -6 from a baculovirus expression system in Sf9 cells. An acetylated fluorogenic peptide,RHKKAc, derived from residues 379-382 of p53 is used as substrate. The reaction buffer is made up of 50 mM Tris-HCl pH 8.0, 127 mM NaCl, 2.7 mM KCl, 1 mM MgCl2, 1 mg/mL BSA, and a final concentration of 1% DMSO. Compounds are delivered in DMSO and delivered to enzyme mixture with preincubation of 5-10 min followed by substrate addition and incubation for 2 h at 30°C. Trichostatin A and developer are added to quench the reaction and generate fluorescence, respectively. Dose-response curves are generated starting at 30 μM compound with three-fold serial dilutions to generate a 10-dose plot. IC50 values are then generated from the resulting plots, and the values expressed are the average of duplicate trials ± standard deviation.
Cell Research	B16 murine melanoma cells are plated at 5000/well in 96 well flat bottom plates. The following day, media is changed to that containing various concentrations of HDACi or matched DMSO vehicle concentrations diluted in complete medium done in triplicate. Cells are incubated for 48 hours at 37°C and 5% CO2. Density of viable, metabolically active cells is quantified using a standard MTS assay as per manufacturer's instructions. Briefly, 20μL of reagent are added per well and incubated at 37°C for 3 hours. Absorbances at 490 nM are measured spectrophotometrically with background subtraction at 690 nM. All values are then normalized and expressed as a percentage of medium control (100%). (Only for Reference)

Solubility Information

Solubility	DMSO: 63 mg/mL (184.53 mM),Sonication is recommended. H2O: < 1 mg/mL (insoluble or slightly soluble), Ethanol: 2 mg/mL (5.86 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (5.86 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.9291 mL	14.6456 mL	29.2912 mL
5 mM	0.5858 mL	2.9291 mL	5.8582 mL
10 mM	0.2929 mL	1.4646 mL	2.9291 mL
50 mM	0.0586 mL	0.2929 mL	0.5858 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

Bergman JA, et al. J Med Chem. 2012, 55(22), 9891-9899.