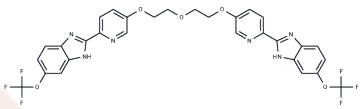
Data Sheet (Cat.No.T6753)

TargetMol

AI-10-49

Chemical Properties



CAS No. : 1256094-72-0

Formula: C30H22F6N6O5

Molecular Weight: 660.52

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	AI-10-49 is a selective inhibitor of the binding of CBFβ-SMMHC to RUNX1 with IC50 of 260 nM.
Targets(IC50)	Others,DNA/RNA Synthesis
In vitro	AI-10-49 displays specific growth inhibition of inv(16)-positive cell line ME-1. AI-10-49 selectively binds to CBFβ-SMMHC, disrupts its binding to RUNX1, and restores RUNX1 transcriptional activity. [1]
In vivo	In mice transplanted with Cbfb+/MYH11;Nras+/G12D leukemic cells, AI-10-49 (200 mg/kg, i.p.) reduces leukemia expansion. [1]
Kinase Assay	FRET assays: Cerulean-Runt domain is expressed and purified. Venus-CBFβ-SMMHC is constructed by inserting 6xHis tag and Venus into pET22b vector between NdeI and NcoI sites, and by inserting CBFβ-SMMHC (the CBFβ-SMMHC construct contains 369 amino acids, 1-166 from CBFβ and 166-369 from MYH11 (amino acids 1526-1730)) between the NcoI and BamHI sites. The fusion protein is purified by standard Ni-affinity chromatography with an on column benzonase treatment to remove residual DNA contaminants. Proteins are dialyzed into FRET buffer (25 mM Tris-HCl, pH 7.5, 150 mM KCl, 2 mM MgCl2) prior to use. Protein concentrations are determined by UV absorbance of the Cerulean and Venus at 433 and 513 nm, respectively. Cerulean-Runt domain and Venus-CBFβ-SMMHC were mixed 1:1 to achieve a final concentration of 10 nM in 96 well black COSTAR plates. DMSO solutions of compounds are added to a final DMSO concentration of 5% (v/v) and the plates incubated at room temperature for one hour in the dark. A PHERAstar microplate reader is used to measure fluorescence (excitation at 433 nm and emission measured at 474 and 525 nm). For IC50 determinations, the ratios of the fluorescence intensities at 525 nm and 474 nm are plotted versus the log of compound concentration, and the resulting curve was fit to a sigmoidal curve using Origin7.0. Three independent measurements are performed and their average and deviation are used for IC50 data fitting.
Cell Research	Cell lines are cultured in IMDM supplemented with 10%~20% fetal bovine serum (FBS) according to culture conditions indicated by ATCC and 1% penicillin/streptomycin (Pen/Strep). All cell lines are tested for mycoplasma. Cells are cultured at 300,000 cells per ml in 96 well plates for 24 and 48 hours in DMSO, or different of AI-10-47, AI-410-49, AI-4-57, or AI-4-88); each in duplicate or triplicate. Cell viability is evaluated using DAPI by flow cytometry. Data is analyzed using FlowJo software and Graphpad Prism

Cell Research	software.(Only for Reference)

Solubility Information

Solubility	Ethanol: 93 mg/mL (140.8 mM),Sonication is recommended. DMSO: 93 mg/mL (140.8 mM),Sonication is recommended. H2O: < 1 mg/mL (insoluble or slightly soluble), (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 3.3 mg/mL (5 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	1.514 mL	7.5698 mL	15.1396 mL
5 mM	0.3028 mL	1.514 mL	3.0279 mL
10 mM	0.1514 mL	0.757 mL	1.514 mL
50 mM	0.0303 mL	0.1514 mL	0.3028 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

Illendula A, et al. Science. 2015, 347(6223), 779-784.