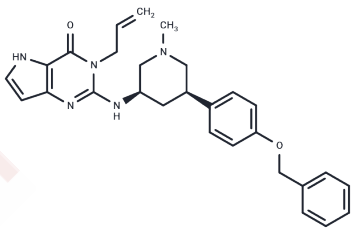
Data Sheet (Cat.No.T9742)

TargetMol

SETDB1-TTD-IN-1

Chemical Properties



CAS No. : 2755823-12-0

Formula: C28H31N5O2

Molecular Weight: 469.58

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	SETDB1-TTD-IN-1 is a potent and selective inhibitor of SET domain bifurcated protein 1 tandem tudor domain (SETDB1-TTD, Kd = 88 nM), and also an endogenous binder competitive inhibitor with a KD of 0.106±0.002 μM for TTD. It can be used to study the biological functions and disease associations of SETDB1-TTD.
Targets(IC50)	Histone Methyltransferase
In vitro	**METHODS**: 16 additional tudor domains were expressed and purified from different tudor domain-containing proteins. **RESULTS** SETDB1-TTD-IN-1 had Kd of 4.3 μM and 86 μM for 53BP1 and JMJD2A, respectively. SETDB1-TTD-IN-1 had no activity against 14 of the tudor domains (KD > 100 mM). [1] **METHODS**: HEK293T cells stably transfected with pLVXmCherry-N1-SETDB1-TTD plasmid were treated with SETDB1-TTD-IN-1 (2.5, 5, 10, 20, 40 μM), and the protein content of the soluble part in the lysate was determined by western blot. **RESULTS** SETDB1-TTD-IN-1 can effectively and dose-dependently stabilize SETDB1-TTD protein in HEK293T cells at a concentration of >= 5 μM.[1]

Solubility Information

Solubility	DMSO: 252.5 mg/mL (537.71 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: 5 mg/mL (10.65 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	2.1296 mL	10.6478 mL	21.2956 mL
5 mM	0.4259 mL	2.1296 mL	4.2591 mL
10 mM	0.213 mL	1.0648 mL	2.1296 mL
50 mM	0.0426 mL	0.213 mL	0.4259 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

Guo Y, et al. Structure-Guided Discovery of a Potent and Selective Cell-Active Inhibitor of SETDB1 Tudor Domain. Angew Chem Int Ed Engl. 2021 Apr 12;60(16):8760-8765.
Uneme Y, Maeda R, Nakayama G, et al.Morc1 reestablishes H3K9me3 heterochromatin on piRNA-targeted transposons in gonocytes.Proceedings of the National Academy of Sciences.2024, 121(13): e2317095121.