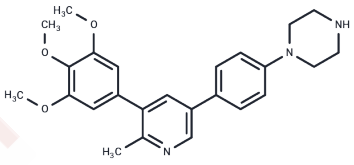
Data Sheet (Cat.No.T1944)

TargetMol

LDN-214117

Chemical Properties



CAS No. : 1627503-67-6

Formula: C25H29N3O3

Molecular Weight: 419.52

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	LDN-214117 is a potent and selective ALK2 inhibitor.
Targets(IC50)	ALK,TGF-beta/Smad
In vivo	LDN-214117 exhibits selective inhibition towards BMP6 over BMP2 or BMP4. In cell-based assays, it preferentially inhibits BMP6 with an IC50 around 100 nM, being 164 times more selective for BMP6 than for TGF-β1. Among kinases, LDN-214117 most effectively inhibits ALK2 (IC50 = 24 nM), followed by TNIK, RIPK2, and ABL1. It specifically inhibits the kinase activity of ALK2 and ALK1 more than that of ALK3.
Kinase Assay	ALK2 kinase assay: Puri?ed recombinant ALK2 proteins, ATP, ATP[γ-32P], and dephosphorylated casein at ?nal concentrations of 2.5 nM, 6 μM, 0.05 μCi/μL , and 0.5 mg/mL, respectively, are aliquoted in kinase bu?er containing 0.2% BSA supplemented with 10 mM MnCl2 into 96-microwell plates, in combination with inhibitor compounds diluted at varying concentrations (0.01 nM to 100 μM). Positive control samples lacking inhibitor compounds, and negative controls lacking recombinant kinase, are also measured. The mixture is reacted at RT for 45 min, quenched with a ?nal concentration of 2% phosphoric acid. The reaction mixture is transferred to 96-well P81 phosphocellulose ?lter plates and bound for 5 min. The plates are washed 20 times with 150 μL of 1% phosphoric acid solution per well by vacuum manifold. Plates are dried at RT for 1 h, sealed, and assayed with Microscint 20 scintillation ?uid using a Spectramax L luminometer. Data is normalized to positive controls at 100% enzyme activity, with negative controls being subtracted as background.
Cell Research	Cells are seeded at 25000 cells per well in 96-well plates and incubated for 2 h at 37°C and 5% CO2. Compounds of LDN-214117 or DMSO are diluted in DMEM and added at ? nal compound concentrations of 1, 10, and 100 μM. Cells are incubated for 4 and 24 h, after which the media is discarded. Cells are lysed by adding 30 μL of passive lysis bu?er and shaken at RT for 15 min. Cell viability is determined by quantifying the ATP present in each well by adding 10 μL of Cell Titer Glo per well and measuring the light output by Spectramax L luminometer. Data is normalized to 100% viability for cells receiving only DMSO.(Only for Reference)

Solubility Information

Solubility	Ethanol: 42 mg/mL (100.11 mM),Sonication is recommended. DMSO: 4.2 mg/mL (10.01 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: 1 mg/mL (2.38 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	2.3837 mL	11.9184 mL	23.8368 mL
5 mM	0.4767 mL	2.3837 mL	4.7674 mL
10 mM	0.2384 mL	1.1918 mL	2.3837 mL
50 mM	0.0477 mL	0.2384 mL	0.4767 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

Mohedas AH, et al. J Med Chem. 2014, 57(19), 7900-7915.