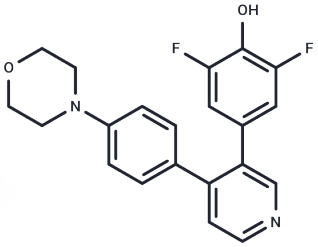
Data Sheet (Cat.No.T6878)

TargetMol

LJI308

Chemical Properties



CAS No. : 1627709-94-7

Formula: C21H18F2N2O2

Molecular Weight: 368.38

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	LJI308 is a potent, and pan-RSK (p90 ribosomal S6 kinase) inhibitor with IC50 of 6 nM, 4 nM, and 13 nM for RSK1, RSK2, and RSK3, respectively.
Targets(IC50)	S6 Kinase,Y Box Binding Protein 1
In vitro	In MDA-MB-231 and H358 cells, LJI308 blocks cellular inhibition of RSK and its phosphorylation of YB1 on Ser102 with EC50 of 0.2-0.3 μM, and thus inhibits cell growth. [1] In TNBC HTRY-LT cells, LJI308 also suppresses cell growth correlative with YB-1 inhibition. [2]
Kinase Assay	Inhibition of RSK1, RSK2, and RSK3 activity: Enzymatic activity of RSK isoforms 1, 2, and 3 is assessed using recombinant full-length RSK protein. RSK1 (1 nM), RSK2 (0.1 nM), or RSK3 (1 nM) is allowed to phosphorylate 200 nM peptide substrate (biotin-AGAGRSRHSSYPAGT-OH) in the presence of ATP at concentration equal to the Km for ATP for each enzyme (RSK1- 5 μM, RSK2- 20 μM, RSK3- 10 μM) and appropriate dilutions of RSK inhibitors in 50 mM HEPES, pH 7.5, 10 mM MgCl2, 1 mM DTT, 0.1% BSA Fraction V, 0.01% Tween-20. After 150 min at room temperature, the reaction is stopped with 60 mM EDTA and extent of peptide phosphorylation was determined using an anti-phospho-AKT substrate antibody and AlphaScreen reagents as described by the manufacturer.
Cell Research	Cell growth under attached conditions is assessed by plating 1000 cells per well on 96-well tissue culture-treated plates in cell growth medium. Appropriate dilutions of compound are 4 added medium above cells and cell growth was assessed after 72 hrs by addition of CellTiter Glo reagent according to manufacturer's directions. (Only for Reference)

Solubility Information

Solubility	H2O: Insoluble, DMSO: 50 mg/mL (135.73 mM),Heating is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Corn Oil: 2.5 mg/mL (6.79 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	2.7146 mL	13.5729 mL	27.1459 mL
5 mM	0.5429 mL	2.7146 mL	5.4292 mL
10 mM	0.2715 mL	1.3573 mL	2.7146 mL
50 mM	0.0543 mL	0.2715 mL	0.5429 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

Aronchik I, et al. Mol Cancer Res. 2014, 12(5), 803-812.
Timosaponin B II as a novel KEAP1-NRF2 inhibitor to alleviate alcoholic liver disease:Receptor structure-based virtual screening and biological evaluation
Davies AH, et al. Oncotarget. 2015, 6(24), 20570-205777.