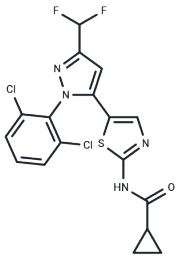
Data Sheet (Cat.No.T4600)

TargetMol

BMS-3

Chemical Properties



CAS No. : 1338247-30-5

Formula: C17H12Cl2F2N4OS

Molecular Weight: 429.27

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	BMS-3 is a potent LIMK inhibitor with IC50 values of 5 nM and 6 nM for LIMK1 and LIMK2, respectively.
Targets(IC50)	LIM Kinase
In vitro	BMS-3 (Compound 2) exhibits a dose-dependent decrease in A549 human lung cancer cell viability by inducing mitotic arrest, characterized by enhanced total nuclear DNA intensity and histone H3 phosphorylation following a 24-hour exposure. It effectively inhibits these cells with an EC50 value of 154 nM[1]. Additionally, BMS-3 elucidates the role of LIMK1 in Cofilin phosphorylation; inhibition of p-LIMK by BMS-3 (1-50 μM) leads to a notable reduction in p-Cofilin levels after a 10-minute incubation under capacitating conditions, with a marked decrease in actin polymerization levels compared to the DMSO controls. Furthermore, under capacitating conditions, mouse sperm exposure to escalating concentrations of BMS-3 (0, 1, 10, and 50 μM) for 90 minutes significantly diminishes the percentage of sperm undergoing acrosomal exocytosis upon Progesterone stimulation[2], highlighting BMS-3's potential in affecting sperm functionality.
Kinase Assay	The protein kinase domains of human LIMK1 and LIMK2 are expressed as glutathione S-transferase fusion proteins using the Bac-to-Bac system in Sf9 cells. Compounds 1 to 6 (e.g., BMS-3) are assayed for inhibition of LIMK1 and LIMK2 protein kinase activity by radioactive phosphate incorporation into biotinylated full-length human destrin. Reactions are done with a concentration series of compound in 25 mM HEPES, 100 mM NaCl, 5 mM MgCl2, 5 mM MnCl2, 1 μM total ATP, 83 μg/mL biotinylated destrin, 167 ng/mL glutathione S-transferase-LIMK1, or 835 ng/mL glutathione S-transferase-LIMK2 in a total volume of 60 μL at room temperature for 30 min (LIMK1) or 60 min (LIMK2). Reactions are terminated by addition of 140 μL of 20% TCA/100 mM sodium pyrophosphate, and the precipitates are harvested onto GF/C unifilter plates. The radioactivity incorporated is determined using a TopCount after addition of 35 μL Microscint scintillation fluid[1]

Solubility Information

Solubility	DMSO: 27.5 mg/mL (64.06 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 (4.66 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	2.3295 mL	11.6477 mL	23.2954 mL
5 mM	0.4659 mL	2.3295 mL	4.6591 mL
10 mM	0.233 mL	1.1648 mL	2.3295 mL
50 mM	0.0466 mL	0.233 mL	0.4659 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

Ross-Macdonald P, et al. Identification of a nonkinase target mediating cytotoxicity of novel kinase inhibitors. Mol Cancer Ther. 2008 Nov;7(11):3490-8.

Romarowski A, et al. PKA-dependent phosphorylation of LIMK1 and Cofilin is essential for mouse sperm acrosomal exocytosis. Dev Biol. 2015 Sep 15;405(2):237-49.