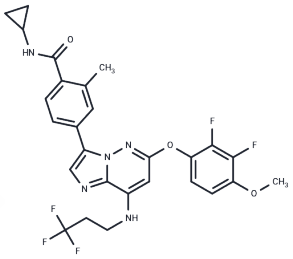
Data Sheet (Cat.No.T3434)

TargetMol

BAY1217389

Chemical Properties



CAS No. : 1554458-53-5

Formula: C27H24F5N5O3

Molecular Weight: 561.5

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	BAY 1217389 is an effective and selective inhibitor of the monopolar spindle 1 (MPS1) kinase (IC50<10 nM).
Targets(IC50)	Kinesin
In vitro	In biochemical assays, the IC50 value of BAY 1217389 is 0.63±0.27 nmol/L. It shows high selectivity against other kinases and found to bind to PDGFRβ (10 nmol/L), Kit (between 10 and 100 nmol/L), CLK1, CLK2, CLK4, JNK1, JNK2, JNK3, LATS1, MAK, MAPKAP2, MERTK, p38β, PDGFRα, PIP5K1C, PRKD1, and RPS6KA5 (between 100 and 1,000 nmol/L). In cellular mechanistic assays, BAY1217389 abrogats nocodazole-induced SAC activity and induced premature exit from mitosis ('mitotic breakthrough'), resulting in multinuclearity and tumor cell death. It is found to inhibit cell proliferation with a median IC50 of 6.7 nmol/L (range 3 to >300 nmol/L)[1].
In vivo	In vivo, BAY 1217389 achieves moderate efficacy in monotherapy in tumor xenograft studies. Its blood clearance is found to be low in the tested species. Vss is high and terminal half-lives were long. BAY 1217389 is administered orally to female NMRI mouse (1 mg/kg) and male Wistar rat (0.5 mg/kg). Peak plasma concentrations are observed between 1.5 and 7 hours. Oral bioavailability is high in rat and moderate in mouse[1].
Kinase Assay	Inhibition of recombinant human Mps1 by BAY 1161909 or BAY 1217389 is assessed in TRFRET-based in vitro kinase assays via phosphorylation of a biotinylated peptide (Biotin-Ahx-PWDPDDADITEILG-NH2). Under standard assay conditions kinase and test compound are preincubated for 15 min before enzyme reaction is started by addition of substrate and ATP upon 10 μM[1].
Cell Research	Cells are seeded into 96-well plates at densities ranging from 1,000 to 5,000 cells per well in the appropriate medium supplemented with 10% FCS. After 24 hours, cells are treated in quadruplicates with serial dilutions of compounds. After further 96 hours, adherent cells are fixed with glutaraldehyde and stained with crystal violet. IC50 values are calculated by means of a 4-parameter fit using the company's own software.(Only for Reference)

Solubility Information

Solubility	DMSO: 30 mg/mL (53.43 mM),Sonication is recommended. H2O: < 1 mg/mL (insoluble or slightly soluble), Ethanol: 3 mg/mL (5.34 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Corn Oil: 3.3 mg/mL (5.88 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	1.7809 mL	8.9047 mL	17.8094 mL
5 mM	0.3562 mL	1.7809 mL	3.5619 mL
10 mM	0.1781 mL	0.8905 mL	1.7809 mL
50 mM	0.0356 mL	0.1781 mL	0.3562 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

Wengner AM, et al. Mol Cancer Ther. 2016, 15(4):583-92.