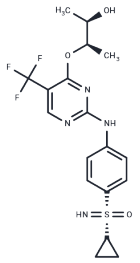
Data Sheet (Cat.No.T16784)

TargetMol

Roniciclib

Chemical Properties



CAS No. : 1223498-69-8

Formula: C18H21F3N4O3S

Molecular Weight: 430.44

Storage: Store at low temperature,Keep away from moisture
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	Roniciclib (BAY 1000394) is a potent pan-CDK inhibitor and a novel oral cytotoxic agent. Roniciclib inhibits the activity of cell-cycle CDKs CDK1, CDK2, CDK3, CDK4, and of transcriptional CDKs CDK7 and CDK9 with IC(50) values in the range between 5 and 25 nmol/L.
Targets(IC50)	CDK
In vitro	Roniciclib inhibits the kinase activity of the cell-cycle CDKs CDK1/cyclin B, CDK2/cyclin E, and CDK4/cyclinD (IC50: 7, 9, and 11 nM, respectively). Roniciclibeffectively inhibits the proliferation of various human and murine tumor cell lines with a very balanced profile (mean IC50 on human tumor cells: 16 nM). The transcriptional CDKs CDK9/cyclin T1 and CDK7/cyclin H/MAT1 are inhibited in a similar range (5 and 25 nM) [1][2].
In vivo	Roniciclib has low blood clearance rates in mouse, rat, and dog (0.51, 0.78, and 0.50 Lh-1kg-1, respectively). Roniciclib strongly inhibits the growth of HeLa-MaTu tumors that have been grown to a size of approximately 50mm2 before the start of treatment. Roniciclib (1.5 and 1 mg/kg) treatment slow tumor growth to T/C values of 0.15 and 0.62, respectively. The addition of Roniciclib to cisplatin causes a strong tumor growth inhibition with T/C values of 0.01 (1.0 mg/kg Roniciclib) and -0.02 (1.5 mg/kg Roniciclib) [1][2].

Solubility Information

Solubility	DMSO: 249 mg/mL (578.48 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 (11.62 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	2.3232 mL	11.616 mL	23.232 mL
5 mM	0.4646 mL	2.3232 mL	4.6464 mL
10 mM	0.2323 mL	1.1616 mL	2.3232 mL
50 mM	0.0465 mL	0.2323 mL	0.4646 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

Siemeister G, et al. BAY 1000394, a novel cyclin-dependent kinase inhibitor, with potent antitumor activity in mono- and in combination treatment upon oral application. Mol Cancer Ther. 2012 Oct;11(10):2265-73.
Lücking U, et al. The lab oddity prevails: discovery of pan-CDK inhibitor (R)-S-cyclopropyl-S-(4-{[4-{[(1R,2R)-2-hydroxy-1-methylpropyl]oxy}-5-(trifluoromethyl)pyrimidin-2-yl]amino}phenyl)sulfoximide (BAY 1000394) for the treatment of cancer. ChemMedChem. 2013 Jul;8(7):1067-85.

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