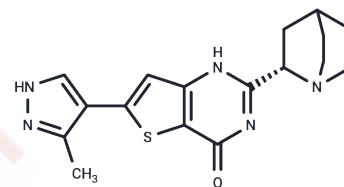


Simurosertib

Chemical Properties

CAS No. :	1330782-76-7
Formula:	C17H19N5OS
Molecular Weight:	341.43
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	Simurosertib (TAK-931) is a selective and ATP-competitive cell division cycle 7 kinase inhibitor (IC50: <0.3 nM).
Targets(IC50)	CDK
In vitro	Simurosertib effectively inhibits CDC7 kinase activity (IC50 0.3 nM) with time-dependent ATP-competitive kinetics to its ATP-binding pocket. Treatment with Simurosertib inhibits the cellular MCM2 phosphorylation at Ser40 in a dose-dependent manner, resulting in a delayed S phase progression, DNA-damage checkpoint activation, and caspase-3/7 activation. The selectivity studies using the 308 kinases reveals >120-fold selectivity of Simurosertib for CDC7 kinase inhibition compared to other kinase inhibitions [1].
In vivo	Simurosertib (p.o.) inhibits pMCM2 of the xenografted COLO205 in a dose- and time-dependent manner in the COLO205-xenograft mouse model. Simurosertib shows a significant antitumor activity in multiple xenograft models [1].

Solubility Information

Solubility	DMSO: 47 mg/mL (137.66 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 (5.86 mM), Sonication is recommended. <i>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.</i>

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.9289 mL	14.6443 mL	29.2886 mL
5 mM	0.5858 mL	2.9289 mL	5.8577 mL
10 mM	0.2929 mL	1.4644 mL	2.9289 mL
50 mM	0.0586 mL	0.2929 mL	0.5858 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

K Iwai, et al. A novel CDC7-selective inhibitor TAK-931 with potent antitumor activity. *European Journal of Cancer* , 2016 , 69 (1) :S34.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

This product is for Research Use Only· Not for Human or Veterinary or Therapeutic Use

Tel:781-999-4286 E_mail:info@targetmol.com Address:34 Washington Street,Wellesley Hills,MA 02481