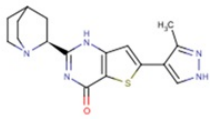
Data Sheet (Cat.No.T12642L)

TargetMol
A DRUG SCREENING EXPERT

Simurosertib

Chemical Properties



CAS No.:	1330782-76-7
Formula:	C17H19N5OS
Molecular Weight:	341.43
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	Simurosertib is a selective and ATP-competitive cell division cycle 7 kinase inhibitor (IC50: <0.3 nM).
Targets(IC_{50})	Cdc7: <0.3 nM
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: 75 mg/mL (219.66 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.929 mL	14.644 mL	29.289 mL
5 mM	0.586 mL	2.929 mL	5.858 mL
10 mM	0.293 mL	1.464 mL	2.929 mL
50 mM	0.059 mL	0.293 mL	0.586 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

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

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