Simurosertib

Cat. No.: HY-100888

CAS No.: 1330782-76-7

Molecular Formula: $C_{17}H_{19}N_5OS$

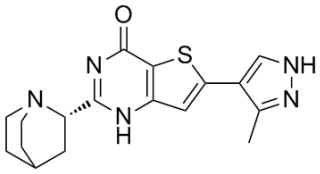
Molecular Weight: 341.43

Target: CDK

Pathway: Cell Cycle/DNA Damage

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 75 mg/mL (219.66 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	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

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 1% DMSO >> 99% saline
   Solubility: ≥ 0.5 mg/mL (1.46 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (7.32 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (7.32 mM); Clear solution
4. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (7.32 mM); Clear solution
5. Add each solvent one by one: 5% DMSO >> 40% PEG300 >> 5% Tween-80 >> 50% saline
   Solubility: ≥ 2.5 mg/mL (7.32 mM); Clear solution
6. Add each solvent one by one: 5% DMSO >> 95% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (7.32 mM); Clear solution

BIOLOGICAL ACTIVITY

Description Simurosertib (TAK-931) is an orally active, selective and ATP-competitive cell division cycle 7 (CDC7) kinase inhibitor, with an

	IC_{50} of <0.3 nM. Simurosertib has anti-cancer activity[1].
IC_{50} & Target	Cdc7 <0.3 nM (IC_{50})
In Vitro	Simurosertib (TAK-931) potently inhibits CDC7 kinase activity (IC_{50} <0.3 nM) with a time-dependent ATP-competitive kinetics to its ATP-binding pocket. The selectivity studies using the 308 kinases reveals >120-fold selectivity of Simurosertib (TAK-931) for CDC7 kinase inhibition compared to other kinase inhibitions. Treatment with Simurosertib (TAK-931) suppresses the cellular MCM2 phosphorylation at Ser40 (pMCM2) in a dose-dependent manner, resulting in a delayed S phase progression, DNA-damage checkpoint activation, and caspase-3/7 activation[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	In the COLO205-xenograft mouse model, oral administration of Simurosertib (TAK-931) inhibits pMCM2 of the xenografted COLO205 in dose- and time-dependent manners. Furthermore, Simurosertib (TAK-931) exhibits a significant antitumor activity in multiple xenograft models[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Nucleic Acids Res. 2020 Aug 20;48(14):7844-7855.
- Breast Cancer Res. 2019 Jul 1;21(1):77.

See more customer validations on www.MedChemExpress.com

REFERENCES

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

India Contact:
Life Technologies (India) Pvt. Ltd.
306, Aggarwal City Mall, Opposite M2K Pitampura, Delhi – 110034 (INDIA). Ph: +91-11-42208000, 42208111, 42208222, Mobile: +91-9810521400, Fax: +91-11-42208444
Email: customerservice@lifetechindia.com Website: www.lifetechindia.com