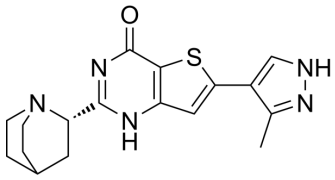
Simurosertib

Cat. No.:	HY-100888
CAS No.:	1330782-76-7
Molecular Formula:	$C_{17}H_{19}N_5OS$
Molecular Weight:	341
Target:	CDK
Pathway:	Cell Cycle/DNA Damage
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 1 year -20°C 6 months



SOLVENT & SOLUBILITY

In Vitro

DMSO : 75 mg/mL (219.94 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.9326 mL	14.6628 mL	29.3255 mL
5 mM	0.5865 mL	2.9326 mL	5.8651 mL
10 mM	0.2933 mL	1.4663 mL	2.9326 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (7.33 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (7.33 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (7.33 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

- Mol Cell. 2021 Sep 7;S1097-2765(21)00683-3.
- Nucleic Acids Res. 2020 Aug 20;48(14):7844-7855.
- J Allergy Clin Immunol. 2023 Feb 24.
- Breast Cancer Res. 2019 Jul 1;21(1):77.
- Cell Death Discov. 2022 Feb 26;8(1):85.

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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.

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