Simurosertib

Cat. No.: HY-100888
CAS No.: 1330782-76-7
Molecular Formula: C₁₇H₁₉N₅OS
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)

<table>
<thead>
<tr>
<th>Preparing Stock Solutions</th>
<th>Solvent Mass</th>
<th>1 mg</th>
<th>5 mg</th>
<th>10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 mM</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5 mM</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10 mM</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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 (7.32 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (7.32 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   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 IC₅₀ of <0.3 nM. Simurosertib has anti-cancer activity[1].

IC₅₀ & Target
Cdc7
<0.3 nM (IC₅₀)
**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\[1\].

**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\[1\].

**CUSTOMER VALIDATION**


See more customer validations on [www.MedChemExpress.com](http://www.MedChemExpress.com)

**REFERENCES**


Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA