SM 16

Cat. No.: HY-111482
CAS No.: 614749-78-9
Molecular Formula: C₂₅H₂₆N₄O₃
Molecular Weight: 430.5
Target: TGF-β Receptor
Pathway: TGF-beta/Smad
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: 65 mg/mL (150.99 mM; Need ultrasonic)

<table>
<thead>
<tr>
<th>Preparing Stock Solutions</th>
<th>Solvent Concentration</th>
<th>Mass</th>
<th>1 mg</th>
<th>5 mg</th>
<th>10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1 mM</td>
<td></td>
<td>2.3229 mL</td>
<td>11.6144 mL</td>
<td>23.2288 mL</td>
</tr>
<tr>
<td></td>
<td>5 mM</td>
<td></td>
<td>0.4646 mL</td>
<td>2.3229 mL</td>
<td>4.6458 mL</td>
</tr>
<tr>
<td></td>
<td>10 mM</td>
<td></td>
<td>0.2323 mL</td>
<td>1.1614 mL</td>
<td>2.3229 mL</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: ≥ 2.58 mg/mL (5.99 mM); Clear solution

2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.58 mg/mL (5.99 mM); Clear solution

3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.58 mg/mL (5.99 mM); Clear solution

BIOLOGICAL ACTIVITY

Description
SM 16 is a ALK5/ALK4 kinase inhibitor with Ki of 10 and 1.5 nM, respectively.

IC₅₀ & Target
Ki: ALK5 (10 nM), ALK4 (1.5 nM)\(^1\)

In Vitro
SM 16 inhibits TGFβ-induced plasminogen activator inhibitor-luciferase activity (IC₅₀=64 nM) and TGFβ- or activin-induced Smad2 phosphorylation at concentrations between 100 and 620 nM. SM 16 is tested against >60 related and
unrelated kinases and shows moderate off-target activity only against Raf (IC$_{50}$=1 μM) and p38/SAPKa (IC$_{50}$=0.8 μM). SM 16 exhibits no inhibitory activity against ALK family members ALK1 and ALK6[1].

**In Vivo**

SM 16 penetrates tumor cells in vivo, suppressing tumor phosphorylated Smad2/3 levels for at least 3 h following treatment of tumor-bearing mice with a single i.p. bolus of 20 mg/kg SM 16. The growth of established AB12 tumors is significantly inhibited by 5 mg/kg/d SM 16 (P<0.001) delivered via s.c. miniosmotic pumps over 28 days[1].

**PROTOCOL**

**Animal Administration**[1]

BALB/c mice are injected on the right flank with 1×10$^6$ AB12 tumor cells. Mice are randomly divided into two groups and one group is implanted with minipumps loaded with 20% Captisol (control) on the left flank and the other group is implanted with minipumps loaded with 20 mg/mL SM 16. Tumor recurrence is defined as the first day when a tumor is unambiguously visible or palpable. Plasma is obtained under anesthesia and analyzed for SM 16[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

**REFERENCES**


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

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