PACMA 31

Cat. No.: HY-100433
CAS No.: 1401089-31-3
Molecular Formula: C₂₁H₂₂N₂O₆S
Molecular Weight: 430.47
Target: Others
Pathway: Others
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 : 100 mg/mL (232.30 mM; Need ultrasonic)

Preparing Stock Solutions
<table>
<thead>
<tr>
<th>Solvent Concentration</th>
<th>Mass 1 mg</th>
<th>Mass 5 mg</th>
<th>Mass 10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 mM</td>
<td>2.3230 mL</td>
<td>11.6152 mL</td>
<td>23.2304 mL</td>
</tr>
<tr>
<td>5 mM</td>
<td>0.4646 mL</td>
<td>2.3230 mL</td>
<td>4.6461 mL</td>
</tr>
<tr>
<td>10 mM</td>
<td>0.2323 mL</td>
<td>1.1615 mL</td>
<td>2.3230 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: ≥ 2.5 mg/mL (5.81 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.81 mM); Clear solution

BIOLOGICAL ACTIVITY

Description
PACMA 31 is an irreversible, orally active protein disulfide isomerase (PDI) inhibitor with an IC₅₀ of 10 μM. PACMA 31 forms a covalent bond with the active site cysteines of PDI. PACMA 31 shows tumor targeting ability and significantly suppresses ovarian tumor growth without causing toxicity to normal tissues[1].

IC₅₀ & Target
IC50: 10 μM (protein disulfide isomerase)[1]

In Vitro
PACMA 31 (0-10 μM; 24 hours) significantly inhibits colony formation in OVCAR-8 cells in a dose-dependent manner[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo
PACMA 31 (20-200 mg/kg; i.p.; daily for 62 days) suppresses tumor growth in human ovarian cancer mouse xenografts[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

**Animal Model:** Athymic mice (bearing OVCAR-8 cells)\(^1\)

**Dosage:** 20-200 mg/kg

**Administration:** I.p., per day for the first 3 wk with 5-d on and 2-d off treatment cycles, and dose was escalated to 40 mg/kg per day for the next 7 d; p.o., the initial dose of 20 mg/kg per day was gradually increased by 20 mg/kg per day with each dose for 3 d before it was orally dosed at 200 mg/kg per day for an additional 32 d, increasing the dose from 20 to 200 mg/kg

**Result:** Compared with the control group, i.p. or per os administration of PACMA 31 significantly inhibited tumor growth by 85% and 65% at day 62, respectively.

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**REFERENCES**