XY101

Cat. No.: HY-128604
CAS No.: 2349368-16-5
Molecular Formula: C₂₅H₂₀F₇NO₄S
Molecular Weight: 563.48
Target: ROR
Pathway: Metabolic Enzyme/Protease
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: 250 mg/mL (443.67 mM; Need ultrasonic)

<table>
<thead>
<tr>
<th>Preparing Stock Solutions</th>
<th>Solvent Concentration</th>
<th>1 mg</th>
<th>5 mg</th>
<th>10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1 mM</td>
<td>1.7747 mL</td>
<td>8.8734 mL</td>
<td>17.7469 mL</td>
</tr>
<tr>
<td></td>
<td>5 mM</td>
<td>0.3549 mL</td>
<td>1.7747 mL</td>
<td>3.5494 mL</td>
</tr>
<tr>
<td></td>
<td>10 mM</td>
<td>0.1775 mL</td>
<td>0.8873 mL</td>
<td>1.7747 mL</td>
</tr>
</tbody>
</table>

In Vivo
1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (3.69 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (3.69 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (3.69 mM); Clear solution

BIOLOGICAL ACTIVITY

Description
XY101 is a potent, selective, metabolically stable and orally available RORγ inverse agonist with an IC₅₀ of 30 nM and a Kᵩ of 380 nM.[1]

IC₅₀ & Target
IC₅₀: 30 nM (RORγ)[1]
Kᵩ: 380 nM (RORγ)[1]
<table>
<thead>
<tr>
<th>In Vitro</th>
<th>XY101 potently inhibits cell growth, colony formation, and the expression of androgen receptor (AR), AR-V7 and prostate-specific antigen (PSA)[^1].</th>
</tr>
</thead>
<tbody>
<tr>
<td>In Vivo</td>
<td>XY101 exhibits significant antitumor activities during the treatment period with tumor growth inhibition and is well tolerated without obvious body weight loss[^1].</td>
</tr>
</tbody>
</table>

**REFERENCES**