XY101

**Cat. No.:** HY-128604  
**CAS No.:** 2349368-16-5  
**Molecular Formula:** C_{25}H_{20}F_{7}NO_{4}S  
**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

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**SOLVENT & SOLUBILITY**

**In Vitro**  
DMSO : 250 mg/mL (443.67 mM; Need ultrasonic)

<table>
<thead>
<tr>
<th>Solvent</th>
<th>Mass</th>
<th>1 mg</th>
<th>5 mg</th>
<th>10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>Preparing Stock Solutions</td>
<td></td>
<td>1 mM</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 mM</td>
<td>1.7747 mL</td>
<td>8.8734 mL</td>
<td>17.7469 mL</td>
<td></td>
</tr>
<tr>
<td>5 mM</td>
<td>0.3549 mL</td>
<td>1.7747 mL</td>
<td>3.5494 mL</td>
<td></td>
</tr>
<tr>
<td>10 mM</td>
<td>0.1775 mL</td>
<td>0.8873 mL</td>
<td>1.7747 mL</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: ≥ 2.08 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

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**BIOLOGICAL ACTIVITY**

**Description**  
XY101 is a potent, selective, metabolically stable and orally available RORγ inverse agonist with an IC_{50} of 30 nM and a K_{d} of 380 nM[1].

**IC_{50} & Target**  
IC50: 30 nM (RORγ)[1]  
Kd: 380 nM (RORγ)[1]

**In Vitro**  
XY101 potently inhibits cell growth, colony formation, and the expression of androgen receptor (AR), AR-V7 and prostate-
specific antigen (PSA)\(^1\).
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

| In Vivo       | XY101 exhibits significant antitumor activities during the treatment period with tumor growth inhibition and is well tolerated without obvious body weight loss\(^1\). MCE has not independently confirmed the accuracy of these methods. They are for reference only. |

**REFERENCES**