# XY101

**Cat. No.:** HY-128604

**CAS No.:** 2349368-16-5

**Molecular Formula:** $C_{25}H_{20}F_7NO_4S$

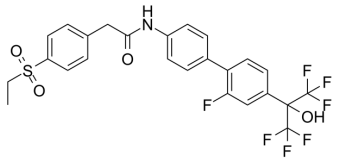
**Molecular Weight:** 563.48

**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)

| Preparing Stock Solutions | Solvent / Mass / Concentration | 1 mg | 5 mg | 10 mg |
|---|---|---|---|---|
| | 1 mM | 1.7747 mL | 8.8734 mL | 17.7469 mL |
| | 5 mM | 0.3549 mL | 1.7747 mL | 3.5494 mL |
| | 10 mM | 0.1775 mL | 0.8873 mL | 1.7747 mL |

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

## 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].<br>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].<br>MCE has not independently confirmed the accuracy of these methods. They are for reference only. |

## REFERENCES

[1]. Zhang Y, et al. Discovery and Characterization of XY101, a Potent, Selective, and Orally Bioavailable RORγ Inverse Agonist for Treatment of Castration-Resistant Prostate Cancer. J Med Chem. 2019 May 9;62(9):4716-4730.

**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