Estrogen receptor β antagonist 2

Cat. No.:	HY-150693			
CAS No.:	2580941-14-4			
Molecular Formula:	$C_{23}H_{26}N_{2}O_{6}$			
Molecular Weight:	426.46			
Target:	Estrogen Receptor/ERR			
Pathway:	Vitamin D Related/Nuclear Receptor			
Storage:	Powder	-20°C	3 years	
		4°C	2 years	
	In solvent	-80°C	6 months	
		-20°C	1 month	

SOLVENT & SOLUBILITY

Pi	DMSO : 100 mg/mL (234.49 mM; Need ultrasonic)							
		Solvent Mass Concentration	1 mg	5 mg	10 mg			
	Preparing Stock Solutions	1 mM	2.3449 mL	11.7244 mL	23.4489 mL			
		5 mM	0.4690 mL	2.3449 mL	4.6898 mL			
		10 mM	0.2345 mL	1.1724 mL	2.3449 mL			
	Please refer to the so	lubility information to select the app	propriate solvent.					
ı Vivo		1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: 2.5 mg/mL (5.86 mM); Clear solution; Need ultrasonic						
		2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: 2.5 mg/mL (5.86 mM); Clear solution; Need ultrasonic						
		3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: 2.5 mg/mL (5.86 mM); Clear solution; Need ultrasonic						

BIOLOGICAL ACTIVITY					
Description	Estrogen receptor β antagonist 2 is a potent and selective estrogen receptor β (ERβ) antagonist with IC ₅₀ s of 109.10, 0.63 μM for Erα and Erβ, respectively ^[1] .				
IC ₅₀ & Target	ERα 109.10 μΜ (IC ₅₀)	ERβ 0.63 μM (IC ₅₀)			
In Vitro	Estrogen receptor β antagonist 2 (compound 42) (0-100 μ M) shows antiproliferative activity with IC ₅₀ value of >100 μ M in				

НО

 NH_2



MCF-7cells^[1].

.Estrogen receptor β antagonist 2 exhibits differences in interaction potential to H₁₂ of ER β via Asp303 (H3) H-bonding to Tyr488^[1].

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

REFERENCES

[1]. Carr M, et al. Optimisation of estrogen receptor subtype-selectivity of a 4-Aryl-4H-chromene scaffold previously identified by virtual screening. Bioorg Med Chem. 2020 Mar 1;28(5):115261.

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

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