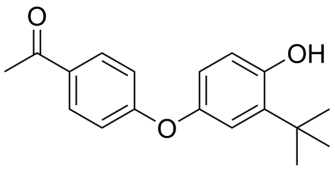
DS45500853

Cat. No.:	HY-132205
CAS No.:	2735803-28-6
Molecular Formula:	$C_{18}H_{20}O_3$
Molecular Weight:	284.35
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

In Vitro

DMSO : 50 mg/mL (175.84 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	3.5168 mL	17.5840 mL	35.1679 mL
	5 mM	0.7034 mL	3.5168 mL	7.0336 mL
	10 mM	0.3517 mL	1.7584 mL	3.5168 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: ≥ 0.5 mg/mL (1.76 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 0.5 mg/mL (1.76 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 0.5 mg/mL (1.76 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

DS45500853 is an estrogen-related receptor α (ERRα) agonist. DS45500853 inhibits the binding between receptor-interacting protein 140 (RIP140) corepressor peptide (10 nM) and GST-ERRα ligand-binding domain (LBD; 1.2 μM) with an IC_{50} value of 0.80 μM. DS45500853 can be used for the research of metabolic disorders, including type 2 diabetes mellitus (T2DM)[1].

IC_{50} & Target

ERRα

In Vitro

DS45500853 (compound 5c; 0.002, 0.006, 0.017, 0.051, 0.015, 0.046, 1.4, 4.2, 12.5 μg/mL; 18 h) activates the transcriptional

activity of full-length ERRα in MG63 cells with an EC_{50} of 5.4 μM[1].
DS45500853 binds in the ligand-binding pocket (LBP) of the ERRα LBD as inverse agonist II[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Shinozuka T, et al. Discovery of a Novel Class of ERRα Agonists. ACS Med Chem Lett. 2021 Apr 21;12(5):817-821.

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