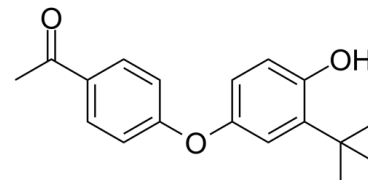


Data Sheet

Product Name:	DS45500853
Cat. No.:	CS-0173281
CAS No.:	2735803-28-6
Molecular Formula:	C ₁₈ H ₂₀ O ₃
Molecular Weight:	284.35
Target:	Estrogen Receptor/ERR
Pathway:	Others
Solubility:	DMSO : 50 mg/mL (175.84 mM; ultrasonic and warming and heat to 60°C)



BIOLOGICAL ACTIVITY:

DS45500853 is an estrogen-related receptor α (**ERR α**) agonist. DS45500853 inhibits the binding between receptor-interacting protein 140 (RIP140) corepressor peptide (10 nM) and GST-ERR α ligand-binding domain (LBD; 1.2 μ M) with an **IC₅₀** value of 0.80 μ M.

DS45500853 can be used for the research of metabolic disorders, including type 2 diabetes mellitus (T2DM)^[1]. **In Vitro:**

DS45500853 (compound 5c; 0.002, 0.006, 0.017, 0.051, 0.015, 0.046, 1.4, 4.2, 12.5 μ g/mL; 18 h) inhibits the transcriptional activity of full-length ERR α in MG63 cells with an EC₅₀ of 5.4 μ M^[1].

DS45500853 binds in the ligand-binding pocket (LBP) of the ERR α LBD as inverse agonist II^[1].

References:

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

CAIndexNames:

1-(4-(3-(Tert-butyl)-4-hydroxyphenoxy)phenyl)ethan-1-one

SMILES:

CC(C1=CC=C(OC2=CC=C(O)C(C(C)(C)C)=C2)C=C1)=O

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

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