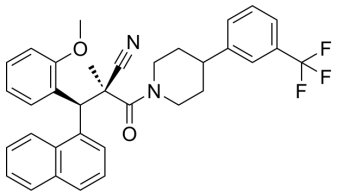
WAY-204688

Cat. No.:	HY-19498
CAS No.:	796854-35-8
Molecular Formula:	$C_{34}H_{31}F_3N_2O_2$
Molecular Weight:	556.62
Target:	NF-κB
Pathway:	NF-κB
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 : 100 mg/mL (179.66 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.7966 mL	8.9828 mL	17.9656 mL
5 mM	0.3593 mL	1.7966 mL	3.5931 mL
10 mM	0.1797 mL	0.8983 mL	1.7966 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (4.49 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

WAY-204688 is an estrogen receptor (ER-α) selective, orally active inhibitor of NF-κB transcriptional activity with an IC_{50} of 122 ± 30 nM for NF-κB-luciferase (NF-κB-luc) in HAECT-1 cells.

IC_{50} & Target

NF-κB-luc 122 nM (IC_{50}, in HAECT-1 cell)	NF-κB

In Vitro

WAY-204688 is ER-dependenrt (activity seen only when hER is coexpressed with NF-κB-luciferase in human aortic endothelial cell lines (HAECT-1) cells). The interaction of WAY-204688 with ERα and ERβ is examined in vitro. WAY-204688 displaces [^{3}H]E2 from the ERα ligand binding domain protein (LBD) with IC_{50}=2.43 μM and from the ERβ ligand binding domain protein (LBD) with IC_{50}=1.5 μM[1].

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

In Vivo	WAY-204688 (5 mg/kg per day, po daily for 5 weeks) is evaluated in vivo for the ability to inhibit four proinflammatory genes (MHC, invariant chain (MHI), VCAM-1, RANTES, and TNF-α). The effect of WAY-204688 on induction of the gene products and on uterine wet weight is compared to that of 17α-ethinyl 17β-estradiol (EE at 10 μg/kg per day) in the same paradigm. Further characterization of WAY-204688 is carried out in several preclinical models of inflammatory disease. In the Lewis rat adjuvant-induced arthritis model (AIA), WAY-204688 is active at a dose of 0.3 mg/kg per day, po[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Caggiano TJ, et al. Estrogen receptor dependent inhibitors of NF-kappaB transcriptional activation-1 synthesis and biological evaluation of substituted 2-cyanopropanoic acid derivatives: pathway selective inhibitors of NF-kappaB, a potential treatment for rheumatoid arthritis. J Med Chem. 2007 Nov 1;50(22):5245-8.

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