Product Datasheet

WAY-204688

Catalog No. **BP-02234** · CAS **796854-35-8** · Form **free base** · Physical state **other** · Color **White to off-white** · Version **1.0** · Revision **2026-09-03**

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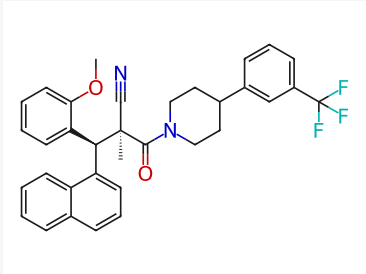
Target	Research area
NF-κB	**Inflammation/Immunology**

Molecular formula	$C_{34}H_{31}F_3N_2O_2$
Molecular weight	**556.6173**

STRUCTURE



DESCRIPTION

WAY-204688 (SIM-688) is an estrogen receptor (ER-α) selective, orally active inhibitor of NF-κB transcriptional activity with an IC50 of 122 ± 30 nM for NF-κB-luciferase (NF-κB-luc) in HAECT-1 cells.

BIOLOGICAL ACTIVITY

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 [3H]E2 from the ERα ligand binding domain protein (LBD) with IC50=2.43 μM and from the ERβ ligand binding domain protein (LBD) with IC50=1.5 μM.

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.

SOLUBILITY

Soluble in DMSO

In vitro	DMSO : 100 mg/mL

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.

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