Product Data Sheet

Product Name: WAY-204688 (SIM-688)
Cat. No.: GC31798

Chemical Properties

Cas. No.	796854-35-8		
SMILES	COC1=C([C@H](C2=CC=CC3=C2C=CC=C3)[C@@](C)(C#N)C(N4CCC(C5=CC(C(F)(F)F)=CC=C5)CC4)=O)C=CC=C1		
Formula	$C_{34}H_{31}F_3N_2O_2$	M.Wt	556.62
Solubility	DMSO : 100 mg/mL (179.66 mM; Need ultrasonic)	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	WAY-204688 (SIM-688)		

Background

WAY-204688 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.

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[1].

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

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com
Address: 10292 Central Ave. #205, Montclair, CA, USA

model (AIA), WAY-204688 is active at a dose of 0.3 mg/kg per day, po[1].

[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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