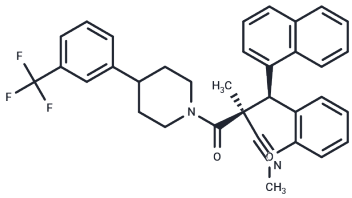
Data Sheet (Cat.No.T17252)

TargetMol
YOUR TARGET MOLECULES

SIM-688

Chemical Properties



CAS No. : 796854-35-8

Formula: C34H31F3N2O2

Molecular Weight: 556.62

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	SIM-688 is a selective and orally active estrogen receptor inhibitor of NF-κB transcriptional activity (IC50 = 122 nM in HAECT-1 cells).
Targets(IC50)	Estrogen/progestogen Receptor,NF-κB
In vitro	SIM-688 displaces [3H]E2 from the ERα ligand-binding domain protein (C50=2.43 μM) and from the ERβ ligand-binding domain protein (IC50=1.5 μM)[1].
In vivo	SIM-688 (5 mg/kg per day, p.o.) inhibits pro-inflammatory genes including MHI, VCAM-1, RANTES, and TNF-α and induces the gene products and uterine wet weight. SIM-688 (0.3 mg/kg, p.o.) is active in the Lewis rat adjuvant-induced arthritis model [1].

Solubility Information

Solubility	DMSO: 90 mg/mL (161.7 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
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
50 mM	0.0359 mL	0.1797 mL	0.3593 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Reference

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-

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