CC-90001

Cat. No.: HY-138304

CAS No.: 1403859-14-2

Molecular Formula: $C_{16}H_{27}N_5O_2$

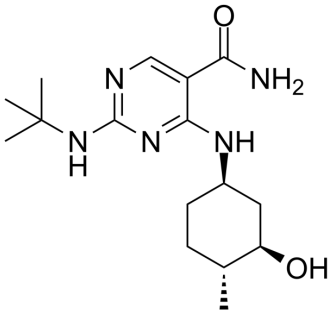
Molecular Weight: 321.42

Target: JNK

Pathway: MAPK/ERK Pathway

Storage:

Powder	-20°C	3 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 125 mg/mL (388.90 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.1112 mL	15.5560 mL	31.1119 mL
	5 mM	0.6222 mL	3.1112 mL	6.2224 mL
	10 mM	0.3111 mL	1.5556 mL	3.1112 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (6.47 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (6.47 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (6.47 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

CC-90001 is a potent, selective and orally active inhibitor of c-Jun N-terminal kinase (JNK). CC-90001 shows 12.9-fold selectivity for JNK1 over JNK2 in a cell-based model. CC-90001 can be used for the research of idiopathic pulmonary fibrosis [1][2].

IC_{50} & Target	JNK1	JNK2

In Vitro

CC-90001 blocks LPS-induced c-jun phosphorylation with an EC_{50} of 480 nM in cellular assays[1].
CC-90001 is 12.9-fold more potent for JNK1 inhibition than JNK2 using JNK1 and JNK2 knockout fibroblasts[1].

	MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	CC-90001 (3 mg/kg b.i.d.) reduces the development of fibrosis, as evidenced by a 48% reduction in collagen and a 53% reduction in α-smooth muscle actin (α-SMA) in a steatohepatitis model[1]. CC-90001 decreases multiple measures of lung collagen and reduces disease induced increases in α-SMA to nearly baseline levels in a house dust mite model of lung fibrosis[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Bennett B, et, al. CC-90001, a Second Generation Jun N-Terminal Kinase (JNK) Inhibitor for the Treatment of Idiopathic Pulmonary Fibrosis. American Journal of Respiratory and Critical Care Medicine 2017; 195:A5409.

[2]. Kolb M, et, al. Therapeutic targets in idiopathic pulmonary fibrosis. Respir Med. 2017 Oct;131:49-57.

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