CC-90005

Cat. No.: HY-132304

CAS No.: 1799574-70-1

Molecular Formula: $C_{21}H_{27}F_2N_7O_2$

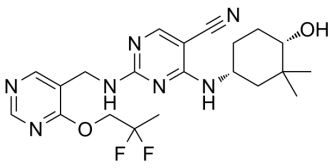
Molecular Weight: 447.48

Target: PKC

Pathway: Epigenetics; TGF-beta/Smad

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 : 62.5 mg/mL (139.67 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.2347 mL	11.1737 mL	22.3474 mL
	5 mM	0.4469 mL	2.2347 mL	4.4695 mL
	10 mM	0.2235 mL	1.1174 mL	2.2347 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: ≥ 1.25 mg/mL (2.79 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 1.25 mg/mL (2.79 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.25 mg/mL (2.79 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

CC-90005 is a potent, selective and orally active inhibitor of protein kinase C-θ (PKC-θ), with an IC_{50} of 8 nM. CC-90005 shows selectivity for PKC-θ over PKC-δ (IC_{50}=4440 nM). CC-90005 can inhibit T cell activation by inhibiting IL-2 expression[1].

IC_{50} & Target

PKCθ
8 nM (IC_{50})

In Vitro

CC-90005 shows the exquisite selectivity of CC-90005, with IC_{50}s for all other family members of >3 μM[1].

CC-90005 is a moderate inhibitor of both CYP2C9 (IC_{50}=8 μM) and CYP2C19 (IC_{50}=5.9 μM) in human liver microsomes[1].
CC-90005 inhibits IL-2 expression in LRS_WBC human PBMCs, with an IC_{50} of 0.15 μM[1].
CC-90005 (1-10 μM; 24 h) inhibits T cell proliferation in PBMCs by 51% at 1 μM and 88% at 3 μM[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

CC-90005 (3-30 mg/kg; p.o. twice daily for 4 days) significantly reduces the popliteal lymph node (PLN) size in a model of chronic T cell activation[1].
CC-90005 (100 mg/kg; a single p.o.) significantly inhibits plasma and spleen IL-2 release by 51 and 54%, respectively[1].
CC-90005 exhibits reasonable oral bioavailability (66 and 46%) and C_{max} (1.18 and 1.2 μM) following oral administration (10 and 3 mg/kg) in rat and dog, respectively[1].
CC-90005 exhibits the mean residence time (0.52 and 2.0 h), CL (69.1 and 20.5 mL/min/kg) and Vss (2.11 and 2.44 L/kg) following intravenous administration (2 and 1 mg/kg) in rat and dog, respectively[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	B6D2F1 mice (20 g) were injected with allogeneic spleen cells
Dosage:	3, 10, 30 mg/kg
Administration:	P.o. twice daily for 4 days
Result:	Inhibited PLN size by 45 and 38% at doses of 10 and 30 mg/kg, respectively.

REFERENCES

[1]. Papa P, et, al. Discovery of the Selective Protein Kinase C-θ Kinase Inhibitor, CC-90005. J Med Chem. 2021 Aug 26;64(16):11886-11903.

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