PD-1/PD-L1-IN-9

Cat. No.: HY-132192

CAS No.: 2628506-54-5

Molecular Formula: $C_{22}H_{24}N_2O_2$

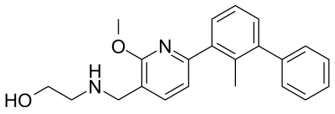
Molecular Weight: 348.44

Target: PD-1/PD-L1

Pathway: Immunology/Inflammation

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 : 100 mg/mL (286.99 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.8699 mL	14.3497 mL	28.6993 mL
	5 mM	0.5740 mL	2.8699 mL	5.7399 mL
	10 mM	0.2870 mL	1.4350 mL	2.8699 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: ≥ 2.5 mg/mL (7.17 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (7.17 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (7.17 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

PD-1/PD-L1-IN-9 is a potent and orally active inhibitor of PD-1/PD-L1 interaction, with an IC_{50} of 3.8 nM. PD-1/PD-L1-IN-9 can enhance the killing activity of tumor cells by immune cells. PD-1/PD-L1-IN-9 also exhibits significant in vivo antitumor activity in a CT26 mouse model[1].

IC_{50} & Target

IC50: 3.8 nM (PD-1/PD-L1)[1]

In Vitro

PD-1/PD-L1-IN-9 (compound 24) (46.9-1500 nM; pretreated for 2 h) dose-dependently significantly activates the antitumor

immunity of peripheral blood mononuclear cells (PBMCs) to MDB-MB 231 cells, with an EC_{50} of -100 nM[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

PD-1/PD-L1-IN-9 (compound 24) (40-80 mg/kg; p.o.; once a day for 2 weeks) inhibits tumor growth in a dose-dependent manner and does not cause any body weight loss or mortality of mice[1].

PD-1/PD-L1-IN-9 (3 mg/kg; i.v.; single dose) exhibits half-life ($T_{1/2}$=4.2 h), plasma clearance (Cl=11.5 L/h/kg) and C_{max} (1233 ng/mL) in rats[1].

PD-1/PD-L1-IN-9 (25 mg/kg; p.o.; single dose) exhibits moderate oral bioavailability (F=22 %), half-life ($t_{1/2}$=6.4 h) and C_{max} (192 ng/mL) in rats[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male BALB/c mice (5-6 weeks) were inoculated CT26 cells[1]
Dosage:	40 mg/kg, 80 mg/kg
Administration:	Oral gavage; once daily, for 2 weeks
Result:	Significantly decreased the final tumor weight, with TGI values of 60 and 67% at the dose of 40 and 80 mg/kg, respectively.

Animal Model:	Pharmacokinetic analysis in sprague-Dawley (SD) rats[1]
Dosage:	3 mg/kg and 25 mg/kg
Administration:	Intravenous injection or oral gavage; single dose

Result:

Route	Dose (mg/kg)	$AUC_{(0-t)}$ (ng·h/mL)	C_{max} (ng/mL)	$t_{1/2}$ (h)	T_{max}	Cl (L·h/kg)	V_z (L/kg)	F (%)
i.v.	3	430.5	1233	4.2	0.03	11.5	78.6	/
p.o.	25	787.4	192	6.4	0.69	28.8	249.3	22

REFERENCES

[1]. Wang T, et, al. Novel Biphenyl Pyridines as Potent Small-Molecule Inhibitors Targeting the Programmed Cell Death-1/Programmed Cell Death-Ligand 1 Interaction. J Med Chem. 2021 May 30.

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