PD-1/PD-L1-IN-9 hydrochloride

Cat. No.: HY-132192A

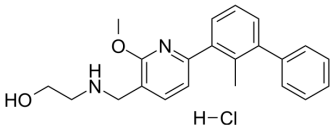
Molecular Formula: $C_{22}H_{25}ClN_2O_2$

Molecular Weight: 384.9

Target: PD-1/PD-L1

Pathway: Immunology/Inflammation

Storage: 4°C, sealed storage, away from moisture
* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 125 mg/mL (324.76 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.5981 mL	12.9904 mL	25.9808 mL
	5 mM	0.5196 mL	2.5981 mL	5.1962 mL
	10 mM	0.2598 mL	1.2990 mL	2.5981 mL

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

BIOLOGICAL ACTIVITY

Description

PD-1/PD-L1-IN-9 hydrochloride 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 hydrochloride can enhance the killing activity of tumor cells by immune cells. PD-1/PD-L1-IN-9 hydrochloride also exhibits significant in vivo antitumor activity in a CT26 mouse model[1].

In Vitro

PD-1/PD-L1-IN-9 hydrochloride (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 hydrochloride (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 hydrochloride (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 hydrochloride (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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