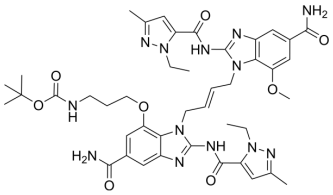
STING agonist-17

Cat. No.:	HY-143320
CAS No.:	2816929-47-0
Molecular Formula:	$C_{43}H_{53}N_{13}O_8$
Molecular Weight:	879.96
Target:	STING
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 (113.64 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.1364 mL	5.6821 mL	11.3642 mL
	5 mM	0.2273 mL	1.1364 mL	2.2728 mL
	10 mM	0.1136 mL	0.5682 mL	1.1364 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 (2.84 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (2.84 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

STING agonist-17 (compound 4a) is a potent STING agonist with an IC_{50} value of 0.062 nM. STING agonist-17 has anti-cancer activity for tumor immunization[1].

IC_{50} & Target

IC_{50}=0.062 nM

In Vitro

STING agonist-17 (compound 4a) inhibits the activity of four major CYP isozymes (CYP1A2, CYP2C9, CYP2C19 and CYP2D6) with IC_{50} values > 100 μM and for CYP3A4 with an IC_{50} = 4.2 μM[1].
STING agonist-17 (compound 4a) (0-2 μM, 24 hours) induces IFN-β secretion with the EC_{50} of 2.0 nM[1].
STING agonist-17 (compound 4a) (2 nM, 10 nM, 6 hours) can induce the expression of signal transduction factors[1].
The pharmacokinetic parameters of Compound 4a in vitro[1].

Parameter	Compound 4a
CYP inhibition (IC50, μM)	
1A2	>100.0
2C9	>100.0
2C19	>100.0
2D6	>100.0
3A4	4.2
Cardiotoxicity (IC50, μM)	
hERG patch clamp assay	>50.0
Liver microsomal phase I stability	
mouse (%)	38.7 ± 2.6
human (%)	11.2 ± 2.7
Plasma stability	
mouse (%)	>99
human (%)	>99

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

Western Blot Analysis[1]

Cell Line:	THP-1 dual cells
Concentration:	2 nM, 10 nM
Incubation Time:	6 hours
Result:	Induced phosphorylation of signal transduction factors STING□TBK1□IRF3 and STAT1 at 2 nM. Activated the expression of IFNB gene and IFN stimulated gene (ISG).

In Vivo

STING agonist-17 (compound 4a) (Intravenous injection; 0.015 mg/kg, 1.5 mg/kg; every other day; a week) has an inhibitory effect on tumor growth in CT26 cells-derived colon carcinoma female BALB/c mice[1].

The pharmacokinetic parameters of Compound 4a in vivo[1].

Parameter	Compound 4a

$T_{1/2}$ (h)	10.54 ± 4.10
Vss (L/kg)	>17.74 ± 5.29
CL (L/h/kg)	2.12 ± 0.27
AUC_{last} (μg•h/mL)	4.20 ± 0.26
AUC_{∞} (μg•h/mL)	>4.78 ± 0.59

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

Animal Model:	Female BALB/c mice aged 6 weeks[1]
Dosage:	0.015 mg/kg, 1.5 mg/kg
Administration:	Intravenous injection; every other day; a week
Result:	Inhibited tumor growth in both doses and caused 57% inhibition at a concentration of 1.5 mg/kg on the 17th day without weight loss.

REFERENCES

[1]. Min Jae Jeon, et al. Development of Potent Immune Modulators Targeting Stimulator of Interferon Genes Receptor. J Med Chem. 2022 Apr 14;65(7):5407-5432.

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