AT791

Cat. No.: HY-124603

CAS No.: 1219962-49-8

Molecular Formula: $C_{23}H_{31}N_3O_3$

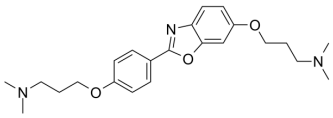
Molecular Weight: 397.51

Target: Toll-like Receptor (TLR)

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 (251.57 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.5157 mL	12.5783 mL	25.1566 mL
5 mM	0.5031 mL	2.5157 mL	5.0313 mL
10 mM	0.2516 mL	1.2578 mL	2.5157 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 (6.29 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.29 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (6.29 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

AT791 is a potent and orally bioavailable TLR7 and TLR9 inhibitor. AT791 inhibits TLR7 and 9 signaling in a variety of human and mouse cell types and inhibits DNA-TLR9 interaction in vitro[1].

IC_{50} & Target

TLR7	TLR9
3.33 μM (IC_{50})	0.04 μM (IC_{50})

In Vitro

AT791 potently suppresses DNA stimulation of HEK:TLR9 cells, with IC_{50} of 0.04 μM and is significantly less effective at

	suppressing R848 stimulation of HEK:TLR7 cells (IC_{50}= 3.33 μM) [1]. AT7916 suppresses TLR9-DNA interaction in vitro, with an IC_{50} in the 1 to10 μM range[1]. AT791 and E6446 are typical of "lysosomotropic"compounds in that they are lipophilic and contain weak base amines. At neutral pH, such compounds are nonpolar and can penetrate lipid membranes, but within low pH vesicles they become protonated and are trapped (de Duve et al., 1974). Capillary electrophoresis showed that AT791 has pK_as of 7.9 and 6.1, and E6446 has pK_as of 8.6 and 6.5, indicating they would be more highly protonated in endolysosomal compartments compared with cytoplasm[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Short-term induction of serum interleukin-6 in mice by CpG1668 DNA is effectively suppresses by pretreatment with AT791 (20 mg/kg; p.o.)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Cell Death Dis. 2023 May 9;14(5):315.

See more customer validations on www.MedChemExpress.com

REFERENCES

[1]. Lamphier M, et al. Novel small molecule inhibitors of TLR7 and TLR9: mechanism of action and efficacy in vivo. Mol Pharmacol. 2014;85(3):429-440.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA