BB-Cl-Amidine hydrochloride

Cat. No.: HY-111347A

CAS No.: 2436747-41-8

Molecular Formula: $C_{26}H_{27}Cl_2N_5O$

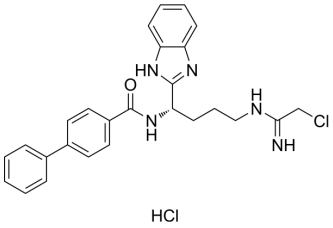
Molecular Weight: 496.43

Target: Protein Arginine Deiminase

Pathway: Epigenetics

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 : 50 mg/mL (100.72 mM; Need ultrasonic)

H_2O : 5 mg/mL (10.07 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.0144 mL	10.0719 mL	20.1438 mL
5 mM	0.4029 mL	2.0144 mL	4.0288 mL
10 mM	0.2014 mL	1.0072 mL	2.0144 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 (5.04 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.04 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.04 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BB-Cl-Amidine hydrochloride is a peptidylarginine deminase (PAD) inhibitor[1].

IC_{50} & Target

PAD[1].

In Vivo

Treatment with BB-Cl-amidine subtly reduces splenomegaly in MRL/lpr mice, while there is a trend towards increased circulating levels of anti-NET antibodies with PAD inhibitor treatment. However, neither PAD inhibitor affected body weight or total IgG levels. Indeed, treatment with both Cl-amidine and BB-Cl-amidine significantly improves endothelium-dependent vasorelaxation. The BB-Cl-amidine group also shows a strong trend towards downregulation of IRGs. Treatment

with either Cl-amidine or BB-Cl-amidine significantly improves muzzle alopecia, in many cases preventing it entirely[1].

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

Animal Model:	MRL/lpr mice[1].
Dosage:	1 mg/kg.
Administration:	Subcutaneous injection daily from 8 to 14 weeks of age.
Result:	Significantly improved endothelium-dependent vasorelaxation and showed a strong trend towards downregulation of IRGs.

CUSTOMER VALIDATION

- Nat Cell Biol. 2021 Oct 6.
- Oncol Rep. 2023 Jul;50(1):146.

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REFERENCES

[1]. Knight JS, et al. Peptidylarginine deiminase inhibition disrupts NET formation and protects against kidney, skin and vascular disease in lupus-prone MRL/lpr mice. Ann Rheum Dis. 2015 Dec;74(12):2199-206.

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