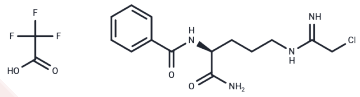
Data Sheet (Cat.No.T10831L2)

TargetMol

Cl-amidine TFA

Chemical Properties



CAS No. : 1043444-18-3

Formula: C16H20ClF3N4O4

Molecular Weight: 424.8

Storage: Store under nitrogen
Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Cl-amidine TFA is an orally active PAD inhibitor with IC_{50} values of 0.8 μM, 6.2 μM and 5.9 μM for PAD1, PAD3 and PAD4, respectively. This compound can induce cancer cell apoptosis, and also upregulate the expression of miR-16 (miRNA-16, microRNA-16), thereby triggering cell cycle arrest. In addition, Cl-amidine TFA can block the citrullination of histone 3 and the formation of neutrophil extracellular traps, effectively improving the survival rate of mice with sepsis.
Targets(IC50)	Apoptosis,PAD,MicroRNA
In vitro	Cl-amidine TFA is a bioavailable haloacetamidine-based compound that inhibits all active PAD isozymes with comparable potency, with an inactivation efficiency constant of 13,000 $M^{-1}\cdot min^{-1}$ for PAD4[1]. When cells are treated with Cl-amidine TFA at concentrations of 0, 5, 10, 15, 20, 25 and 50 μg/mL for 24 hours, it induces apoptosis in TK6 lymphoblastoid cells and HT29 colon cancer cells in a dose-dependent manner; notably, the HT29 colon cancer cell line exhibits relative resistance to apoptosis induced by Cl-amidine[2]. Cl-amidine TFA achieves irreversible inactivation of PADs by covalently modifying the cysteine residue in the PAD active site that is involved in catalytic activity[4].
In vivo	At a dose of 75 mg/kg administered intraperitoneally once daily, Cl-amidine TFA exerts inhibitory and therapeutic effects on dextran sulfate sodium-induced colitis in mice[2]. When administered by oral gavage at doses of 5, 25 and 75 mg/kg once daily, Cl-amidine TFA also significantly reduces the histological scores in a dose-dependent manner[2].

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.354 mL	11.7702 mL	23.5405 mL
5 mM	0.4708 mL	2.354 mL	4.7081 mL
10 mM	0.2354 mL	1.177 mL	2.354 mL
50 mM	0.0471 mL	0.2354 mL	0.4708 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Yuan Luo, et al. Inhibitors and Inactivators of Protein Arginine Deiminase 4: Functional and Structural Characterization. Biochemistry. 2006 Oct 3; 45(39): 11727–11736.
Chumanevich AA, et al. Suppression of colitis in mice by Cl-amidine: a novel peptidylarginine deiminase inhibitor. Am J Physiol Gastrointest Liver Physiol. 2011 Jun;300(6):G929-38.
Witalison EE, et al. Molecular targeting of protein arginine deiminases to suppress colitis and prevent colon cancer. Oncotarget. 2015 Nov 3;6(34):36053-62.
Biron BM, et al., Cl-Amidine Prevents Histone 3 Citrullination and Neutrophil Extracellular Trap Formation, and Improves Survival in a Murine Sepsis Model. J Innate Immun. 2017;9(1):22-32.
Bryan Knuckley, et al. Substrate Specificity and Kinetic Studies of PADs 1, 3, and 4 Identify Potent and Selective Inhibitors of Protein Arginine Deiminase 3. Biochemistry. 2010 Jun 15;49(23):4852-63.