

Cl-amidine TFA

Chemical Properties

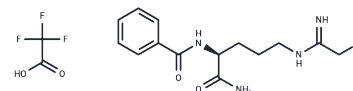
CAS No. : 1043444-18-3

Formula: C₁₆H₂₀ClF₃N₄O₄

Molecular Weight: 424.8

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year



Biological Description

Description	Cl-amidine TFA is an orally active inhibitor of peptidyl arginine deiminase (PAD) (IC ₅₀ s: 0.8 μM, 6.2 μM, and 5.9 μM for PAD1, PAD3, and PAD4). Cl-amidine induces apoptosis in cancer cells.
Targets(IC ₅₀)	Others
In vitro	Cl-amidine TFA inhibits all the active PAD isozymes with near equal potency (kinact/K _i =13,000/(M?min) for PAD4) [1]. Cl-amidine (0, 5, 10, 15, 20, 25, 50 μg/mL, 24 hours) induces apoptosis in TK6 lymphoblastoid cells and HT29 colon cancer cells in a dose-dependent manner. Interestingly, the colon cancer cell line (HT29) is relatively resistant to apoptosis caused by Cl-amidine [2]. Cl-amidine irreversibly inactivates PADs by covalently modifying an active site cysteine that is important for its catalytic activity [4].
In vivo	Cl-amidine (75 mg/kg, i.p. once daily) suppresses and treats DSS-induced colitis in mice. Cl-amidine (5, 25, 75 mg/kg, oral gavage, once daily) leads to significant reductions in the histology scores dose-dependently [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.

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.

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