D-Cl-amidine hydrochloride

Cat. No.: HY-100574D Molecular Formula: $C_{14}H_{20}Cl_2N_4O_2$ Molecular Weight: 347.24

Target: Protein Arginine Deiminase; Apoptosis

Pathway: Epigenetics; Apoptosis

Storage: -20°C, protect from light, stored under nitrogen

* In solvent: -80°C, 6 months; -20°C, 1 month (protect from light, stored under

nitrogen)

Product Data Sheet

SOLVENT & SOLUBILITY

In Vitro

DMSO: 80 mg/mL (230.39 mM; ultrasonic and warming and heat to 60°C) H₂O: 16.67 mg/mL (48.01 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg	
	1 mM	2.8799 mL	14.3993 mL	28.7985 mL	
	5 mM	0.5760 mL	2.8799 mL	5.7597 mL	
	10 mM	0.2880 mL	1.4399 mL	2.8799 mL	

Please refer to the solubility information to select the appropriate solvent.

In Vivo

- 1. Add each solvent one by one: PBS Solubility: 10 mg/mL (28.80 mM); Clear solution; Need ultrasonic
- 2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.67 mg/mL (7.69 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.67 mg/mL (7.69 mM); Clear solution
- 4. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.67 mg/mL (7.69 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	D-Cl-amidine hydrochloride is a potent and highly selective PAD1 inhibitor. D-Cl-amidine is well-torelated with no significant toxicity $^{[1]}$.
In Vitro	D-Cl-amidine (200-400 μ M) is effective in significantly decreasing cell viability in MDA-MB-231 cells ^[1] . D-Cl-amidine increase caspase 3 activity, indicating that inhibition of PAD1 leads to an increase in apoptosis ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

D-Cl-amidine, administered by iv at a dose of 2.5 mg/kg, is still detected after 2 h in serum at a concentration of ~21 nM and at 4 h at ~10 nM. D-Cl-amidine is still observed in the blood serum at a concentration of -10 nM at 4 h when administered by ip at a dose of 10 mg/kg $^{[1]}$.

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[1]. Bicker KL, et al. D-amino acid based protein arginine deiminase inhibitors: Synthesis, pharmacokinetics, and in cellulo efficacy. ACS Med Chem Lett. 2012 Oct 26;3(12):1081-1085.

Caution: Product has not been fully validated for medical applications. For research use only.

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