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Cl-Amidine

Inhibits protein-arginine deiminase (PAD)

Catalog #100-0518 1 mg

Catalog #100-0519 5 mg

Product Description

Cl-Amidine is a protein-arginine deiminase (PAD) inhibitor that irreversibly inactivates four subtypes of PAD (k_{inact}/K_i = 37,000/PAD1, 1,200/PAD2, 2,000/PAD3, and 13,000/PAD4 $M^{-1}min^{-1}$; Knuckley et al.; Luo et al.; Slack et al.) by modifying the enzyme's active site. This product is supplied as the hydrochloride salt of the molecule.

Molecular Name: Cl-Amidine (Hydrochloride)

Alternative Names: Not applicable

CAS Number (Model): 1373232-26-8

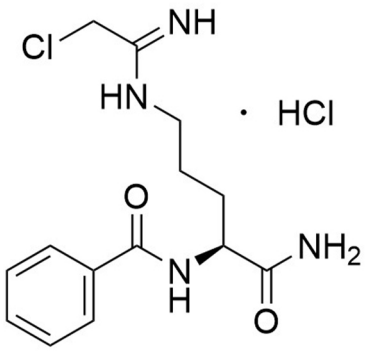
Chemical Formula: $C_{14}H_{19}ClN_4O_2 \bullet HCl$

Molecular Weight: 347.2 g/mol

Purity: ≥ 95%

Chemical Name: N-[(1S)-1-(aminocarbonyl)-4-[(2-chloro-1-iminoethyl)amino]butyl]-benzamide, monohydrochloride

Structure:



Properties

Product Format: A crystalline solid

Stability and Storage: Product stable at -20°C as supplied. As a precaution, STEMCELL recommends storing all small molecules away from direct light. For long-term storage, store with a desiccant. Stable as supplied for 12 months from date of receipt.

Preparation: Solubility:
- PBS (pH 7.2) ≤ 8.6 mM
- DMSO ≤ 140 mM
- Absolute ethanol ≤ 55 mM

For example, to prepare a 10 mM stock solution in DMSO, resuspend 1 mg in 288 µL of DMSO.

Prepare stock solution fresh before use. Information regarding stability of small molecules in solution has rarely been reported, however, as a general guide we recommend storage in DMSO at -20°C. Aliquot into working volumes to avoid repeated freeze-thaw cycles. The effect of storage of stock solution on compound performance should be tested for each application.

For use as a cell culture supplement, stock solution should be diluted into culture medium immediately before use. Avoid final DMSO or absolute ethanol concentration above 0.1% due to potential cell toxicity.

Published Applications

IMMUNOLOGY
· Inhibits neutrophil extracellular traps formation in neutrophils (Knight et al.).
· Prevents hypercitrullination of histone H3 in neutrophils (Knight et al.).
CANCER RESEARCH
· Exhibits cytotoxic effects toward human leukemia (IC50 = 0.25 µM), breast (IC50 = 0.05 µM), and colon (IC50 = 1 µM) cancer cell lines (Slack et al.).

References

Knight JS et al. (2013) Peptidylarginine deiminase inhibition is immunomodulatory and vasculoprotective in murine lupus. J Clin Invest 123(7): 2981–93.

Knuckley B et al. (2010) Substrate specificity and kinetic studies of PADs 1, 3, and 4 identify potent and selective inhibitors of protein arginine deiminase 3. Biochemistry 49(23): 4852–63.

Luo Y et al. (2006) Inhibitors and inactivators of protein arginine deiminase 4: functional and structural characterization. Biochemistry 45(39): 11727–36.

Slack JL et al. (2011) Protein arginine deiminase 4: a target for an epigenetic cancer therapy. Cell Mol Life Sci 68(4): 709–20.

Related Products

For a complete list of small molecules available from STEMCELL Technologies, visit www.stemcell.com/smallmolecules or contact us at techsupport@stemcell.com.

Warning

This product is hazardous. Please refer to the Safety Data Sheet (SDS).