Small Molecules

BB-Cl-Amidine

Inhibits protein-arginine deiminase (PAD)

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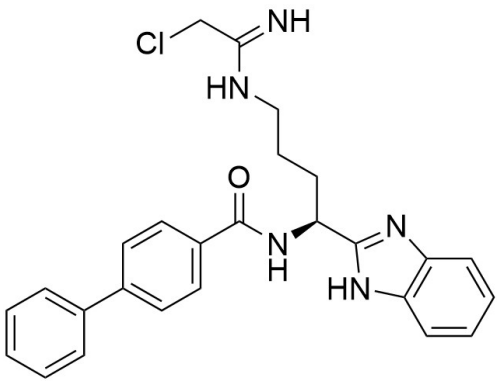
Catalog #100-0516	1 mg
100-0517	5 mg

Product Description

BB-Cl-Amidine is a protein-arginine deiminase (PAD) inhibitor that irreversibly inhibits four subtypes of PAD (k_{inact}/K_i = 16,100/PAD1, 4100/PAD2, 6800/PAD3, and 13,300/PAD4 $M^{-1}min^{-1}$; Luo et al.; Muth et al.). BB-Cl-Amidine is less susceptible to proteolysis than Cl-amidine due to the addition of benzimidazole on its C-terminus (Knight et al.).

Molecular Name:	BB-Cl-Amidine
Alternative Names:	Not applicable
CAS Number:	1802637-39-3
Chemical Formula:	$C_{26}H_{26}ClN_5O$
Molecular Weight:	460.0 g/mol
Purity:	≥ 95%
Chemical Name:	N-[(1S)-1-(1H-benzimidazol-2-yl)-4-[(2-chloro-1-iminoethyl)amino]butyl]-[1,1'-biphenyl]-4-carboxamide
Structure:	



Properties

Physical Appearance:	A crystalline solid
Storage:	Product stable at -20°C as supplied. Protect product from prolonged exposure to light. For long-term storage, store with a desiccant. Stable as supplied for 12 months from date of receipt.
Solubility:	• DMSO ≤ 40 mM • Absolute ethanol ≤ 50 mM For example, to prepare a 10 mM stock solution in DMSO, resuspend 0.5 mg in 109 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. Compound has low solubility in aqueous media. For use as a cell culture supplement, stock solution should be diluted into culture medium immediately before use. Avoid final DMSO concentration above 0.1% due to potential cell toxicity.

Published Applications

IMMUNOLOGY
· Inhibits neutrophil extracellular traps formation in neutrophils (Knight et al.).

References

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

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

Muth A et al. (2017) Development of a selective inhibitor of protein arginine deiminase 2. J Med Chem 60(7): 3198–211.

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