

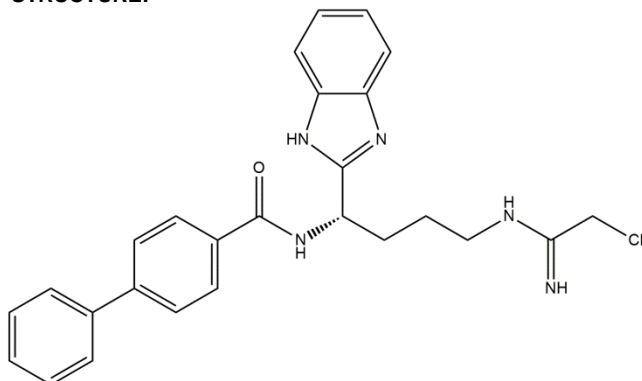
BB-Cl-Amidine

08/19

ALTERNATE NAMES: N-[4-[(1-amino-2-chloroethylidene)amino]-1-(1H-benzimidazol-2-yl)butyl]-4-phenylbenzamide; N-[(1S)-1-(1H-benzimidazol-2-yl)-4-[(2-chloro-1-iminoethyl)amino]butyl]-[1,1'-biphenyl]-4-carboxamide

CATALOG #: B2847-1 1 mg
B2847-5 5 mg

STRUCTURE:



MOLECULAR FORMULA: C₂₆H₂₆ClN₅O

MOLECULAR WEIGHT: 459.97

CAS NUMBER: 1802637-39-3

APPEARANCE: A crystalline solid

PURITY: ≥95%

SOLUBILITY: ~25 mg/ml in ethanol
~20 mg/ml in DMSO and DMF

DESCRIPTION: BB-Cl-Amidine is a pan-peptidylarginine deiminase (PAD) inhibitor. Peptidylarginine deiminase catalyzes the hydrolysis of peptidyl-arginine to form peptidyl-citrulline. BB-Cl-Amidine is a derivative of the PAD inhibitor Cl-amidine in which the C-terminal carboxamide is replaced with a benzimidazole moiety to reduce proteolysis. The cellular potency of BB-Cl-amidine is 20-fold higher than Cl-amidine. The EC₅₀ value for inhibition of viability of U2OS osteosarcoma cells is 8.8 μM. It improves endothelium-dependent vasorelaxation in MRL/lpr mice. It inhibits the formation of neutrophil extracellular traps without altering H₂O₂ production by neutrophils.

STORAGE TEMPERATURE: -20°C

REFERENCES:

1. Knight, J.S., Subramanian, V., O'Dell, A.A., et al. Peptidylarginine deiminase inhibition disrupts NET formation and protects against kidney, skin and vascular disease in lupus-prone MRL/lpr mice. *Annals of the Rheumatic Diseases* 74(12), 2199-2206 (2015).
2. Muth, A., Subramanian, V., Beaumont, E., et al. Development of a selective inhibitor of protein arginine deiminase 2. *J. Med. Chem.* 60(7), 3198-3211 (2017).

HANDLING: Do not take internally. Wear gloves and mask when handling the product! Avoid contact by all modes of exposure.

RELATED PRODUCTS:

F-Amidine (trifluoroacetate salt) (Cat. No. B2803)
Cl-Amidine (hydrochloride) (Cat. No. B2802)
GSK-199 hydrochloride (Cat. No. B1037)
GSK-121 trifluoroacetate (Cat. No. B1034)
GSK-106 hydrochloride (Cat. No. B1036)

DISCLAIMER: **FOR RESEARCH USE ONLY! Not to be used on humans.**