



# SZABO SCANDIC

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## Produktinformation



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- Expressversand

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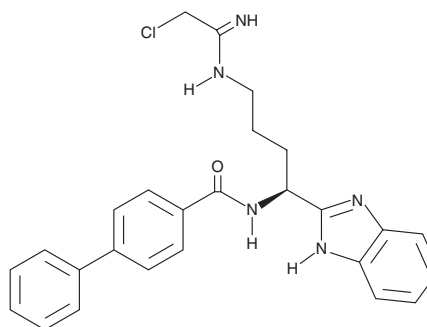
# PRODUCT INFORMATION



## BB-Cl-Amidine

Item No. 17079

**CAS Registry No.:** 1802637-39-3  
**Formal Name:** N-[(1S)-1-(1H-benzimidazol-2-yl)-4-[(2-chloro-1-iminoethyl)amino]butyl]-[1,1'-biphenyl]-4-carboxamide  
**MF:** C<sub>26</sub>H<sub>26</sub>ClN<sub>5</sub>O  
**FW:** 460.0  
**Purity:** ≥95%  
**UV/Vis.:** λ<sub>max</sub>: 274, 281 nm  
**Supplied as:** A crystalline solid  
**Storage:** -20°C  
**Stability:** ≥2 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

### Laboratory Procedures

BB-Cl-Amidine is supplied as a crystalline solid. A stock solution may be made by dissolving the BB-Cl-Amidine in the solvent of choice. BB-Cl-Amidine is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide, which should be purged with an inert gas. The solubility of BB-Cl-Amidine in ethanol is approximately 25 mg/ml and approximately 20 mg/ml in DMSO and DMF.

BB-Cl-Amidine is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, an ethanolic solution of BB-Cl-Amidine should be diluted with the aqueous buffer of choice. BB-Cl-Amidine has a solubility of approximately 0.5 mg/ml in a 1:1 solution of ethanol:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

### Description

BB-Cl-Amidine is a modified version of Cl-amidine (Item No. 10599) that retains the functional components but possesses a C-terminal benzimidazole group designed to limit proteolysis of the C-terminal amide.<sup>1</sup> BB-Cl-Amidine irreversibly inactivates all four PAD subtypes ( $k_{\text{inact}}/K_i = 16,100, 4,100, 6,800$ , and  $13,300 \text{ M}^{-1}\text{min}^{-1}$  for PAD1-4, respectively) by covalently modifying an active site cysteine that is important for its catalytic activity.<sup>2,3</sup> The cellular potency of BB-Cl-amidine against PAD4 is increased 20-fold over the parent compound ( $\text{EC}_{50} = 8.8 \text{ } \mu\text{M}$  versus  $>200 \text{ } \mu\text{M}$  for Cl-amidine). BB-Cl-Amidine also has a significantly longer *in vivo* half-life than Cl-amidine (1.75 h versus ~15 min, respectively). Both compounds inhibit the formation of neutrophil extracellular traps without altering  $\text{H}_2\text{O}_2$  production by neutrophils.<sup>1</sup> BB-Cl-Amidine is effective *in vivo*, improving endothelial function while downregulating the expression of type I interferon-regulated genes in MRL/lpr mice.

### 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. *Ann. Rheum. Dis.* **74**(12), 2199-2206 (2015).
2. Luo, Y., Arita, K., Bhatia, M., *et al.* Inhibitors and inactivators of protein arginine deiminase 4: Functional and structural characterization. *Biochem.* **45**(39), 11727-11736 (2006).
3. 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).

#### WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

#### SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the [complete](#) Safety Data Sheet, which has been sent via email to your institution.

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