

# PRODUCT INFORMATION



## BB-Cl-Amidine (trifluoroacetate salt)

Item No. 17079

**Formal Name:** N-[(1S)-1-(1H-benzimidazol-2-yl)-4-[(2-chloro-1-iminoethyl)amino]butyl]-[1,1'-biphenyl]-4-carboxamide, trifluoroacetate salt

**MF:** C<sub>26</sub>H<sub>26</sub>ClN<sub>5</sub>O • XCF<sub>3</sub>COOH

**FW:** 460.0

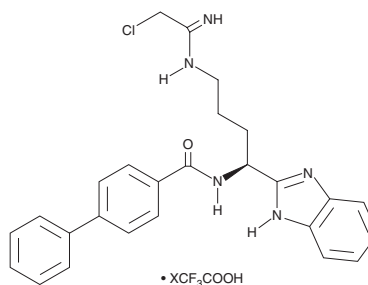
**Purity:** ≥95%

**UV/Vis.:** λ<sub>max</sub>: 274, 281 nm

**Supplied as:** A crystalline solid

**Storage:** -20°C

**Stability:** ≥4 years



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

### Laboratory Procedures

BB-Cl-amidine (trifluoroacetate salt) is supplied as a crystalline solid. A stock solution may be made by dissolving the BB-Cl-amidine (trifluoroacetate salt) in the solvent of choice. BB-Cl-amidine (trifluoroacetate salt) 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 (trifluoroacetate salt) in ethanol is approximately 25 mg/ml and approximately 20 mg/ml in DMSO and DMF.

BB-Cl-amidine (trifluoroacetate salt) is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, an ethanolic solution of BB-Cl-amidine (trifluoroacetate salt) should be diluted with the aqueous buffer of choice. BB-Cl-amidine (trifluoroacetate salt) 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 pan inhibitor of peptidyl arginine deiminases (PADs) and a proteolysis-resistant derivative of Cl-amidine (Item No. 10599).<sup>1</sup> It irreversibly inhibits PAD1-4 ( $k_{\text{inact}}/K_i = 16,100, 4,100, 6,800,$  and  $13,300 \text{ M}^{-1}\text{min}^{-1}$ , respectively).<sup>2,3</sup> BB-Cl-amidine (20 and 200  $\mu\text{M}$ ) inhibits the formation of neutrophil extracellular traps (NETs) induced by phorbol 12-myristate 13-acetate (PMA; Item No. 10008014) without altering hydrogen peroxide ( $\text{H}_2\text{O}_2$ ) production in bone marrow-derived neutrophils.<sup>1</sup> It inhibits IFN- $\beta$  production induced by the DNA virus herpes simplex virus 1 (HSV-1) but not the RNA virus Sendai virus in mouse bone marrow-derived macrophages (BMDMs) when used at a concentration of 1  $\mu\text{M}$ .<sup>4</sup> *Ex vivo*, BB-Cl-amidine (10 mg/kg) reduces BMDM IFN- $\beta$  and TNF- $\alpha$  production induced by diABZI STING agonist-1 (Item No. 28054) in wild-type, *Pad2*<sup>-/-</sup>, and *Pad4*<sup>-/-</sup> mice. BB-Cl-amidine (20 mg/kg per day) increases survival, as well as reduces splenomegaly, myocarditis, and cardiac fibrosis in a Trex1<sup>D18N/D18N</sup> mouse model of Aicardi-Goutières syndrome (AGS).

### 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).
4. Humphries, F., Shmuel-Galia, L., Jiang, Z., *et al.* Targeting STING oligomerization with small-molecule inhibitors. *Proc. Natl. Acad. Sci. USA* **120**(33), e2305420120 (2023).

#### 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.

#### WARRANTY AND LIMITATION OF REMEDY

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#### CAYMAN CHEMICAL

1180 EAST ELLSWORTH RD  
ANN ARBOR, MI 48108 · USA

PHONE: [800] 364-9897

[734] 971-3335

FAX: [734] 971-3640

CUSTSERV@CAYMANCHEM.COM

WWW.CAYMANCHEM.COM