

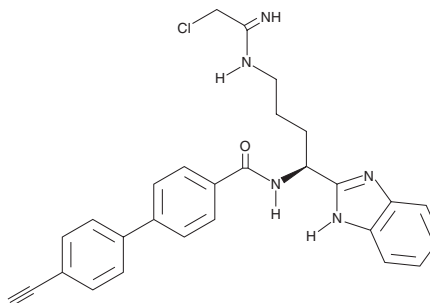
# PRODUCT INFORMATION



## BB-Cl-Yne

Item No. 25378

**CAS Registry No.:** 2219324-71-5  
**Formal Name:** N-[(1S)-1-(1H-benzimidazol-2-yl)-4-[(2-chloro-1-iminoethyl)amino]butyl]-4'-ethynyl-[1,1'-biphenyl]-4-carboxamide  
**Synonym:** Click Tag™ BB-Cl-Yne  
**MF:** C<sub>28</sub>H<sub>26</sub>ClN<sub>5</sub>O  
**FW:** 484.0  
**Purity:** ≥98%  
**UV/Vis.:** λ<sub>max</sub>: 282 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-Yne is supplied as a crystalline solid. A stock solution may be made by dissolving the BB-Cl-Yne in the solvent of choice, which should be purged with an inert gas. BB-Cl-Yne is soluble in organic solvents such as DMSO and dimethyl formamide (DMF). The solubility of BB-Cl-Yne in these solvents is approximately 5 and 20 mg/ml, respectively.

BB-Cl-Yne is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, BB-Cl-Yne should first be dissolved in DMF and then diluted with the aqueous buffer of choice. BB-Cl-Yne has a solubility of approximately 0.16 mg/ml in a 1:5 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

### Description

BB-Cl-Yne is a cell-permeable derivative of the protein arginine deiminase (PAD) inhibitor BB-Cl-amidine (Item No. 17079) that contains an alkyne moiety for use in click chemistry reactions.<sup>1</sup> BB-Cl-Yne inhibits PAD1-4 with  $k_{inact}/K_i$  values of 6,400, 3,600, 10,800, and 4,900 M<sup>-1</sup>min<sup>-1</sup>, respectively. It has been used for labeling PADs in cell-free and cell-based assays, followed by click reactions with azide-modified TAMRA reporters or biotin capture reagents.

### Reference

1. Nemmara, V.V., Subramanian, V., Muth, A., *et al.* The development of benzimidazole-based clickable probes for the efficient labeling of cellular protein arginine deiminases (PADs). *ACS Chem. Biol.* **13**(3), 712-722 (2018).

#### 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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