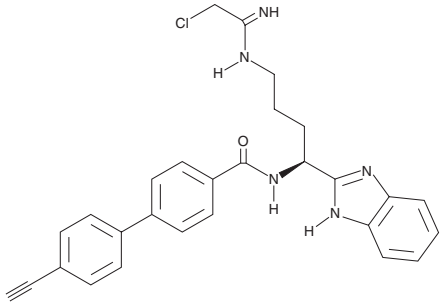
PRODUCT INFORMATION

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:	$C_{28}H_{26}ClN_5O$
FW:	484.0
Purity:	≥98%
UV/Vis.:	λ_{max}: 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.[1] BB-Cl-Yne inhibits PAD1-4 with k_{inact}/K_I values of 6,400, 3,600, 10,800, and 4,900 $M^{-1}min^{-1}$, 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).

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