

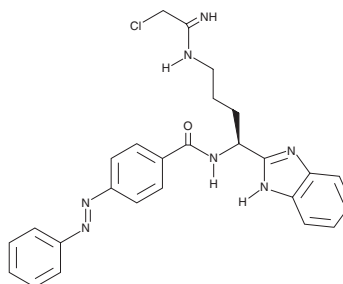
# PRODUCT INFORMATION



## Photoswitchable PAD Inhibitor (technical grade)

Item No. 28104

**CAS Registry No.:** 2226393-62-8  
**Formal Name:** N-[(1S)-1-(1H-benzimidazol-2-yl)-4-[(2-chloro-1-iminoethyl)amino]butyl]-4-(2-phenyldiazenyl)-benzamide  
**MF:** C<sub>26</sub>H<sub>26</sub>ClN<sub>7</sub>O  
**FW:** 488.0  
**Purity:** ≥70% (mixture of isomers)  
**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

Photoswitchable PAD inhibitor (technical grade) is supplied as a crystalline solid. A stock solution may be made by dissolving the photoswitchable PAD inhibitor (technical grade) in the solvent of choice, which should be purged with an inert gas. Photoswitchable PAD inhibitor (technical grade) is soluble in the organic solvent methanol at a concentration of approximately 30 mg/ml.

### Description

Photoswitchable PAD inhibitor is a photoactivated protein arginine deiminase (PAD) inhibitor and a derivative of BB-Cl-amidine (Item No. 17079) that contains an azobenzene photoswitch allowing optical control of PAD activity.<sup>1</sup> Without photoactivation, it is a weak inhibitor of PAD2 (IC<sub>50</sub> = >100 μM) and is less potent than BB-Cl-amidine in inhibiting citrulline production *in vitro* (k<sub>inact</sub>/K<sub>iS</sub> = 2,300, 600, 1,000, and 10,510 M<sup>-1</sup>min<sup>-1</sup> for PAD1-4, respectively) and does not inhibit histone H3 citrullination in HEK293T cells overexpressing PAD2 when used at concentrations up to 100 μM. However, it can rapidly be photoactivated with UV-A radiation to the more active *cis*-isomer, which is an irreversible, competitive inhibitor of histone H3 citrullination with an IC<sub>50</sub> value of 9.1 μM.

### Reference

1. Mondal, S., Parekar, S.S., Nagar, M., *et al.* Photochemical control of protein arginine deiminase (PAD) activity. *ACS Chem. Biol.* **13**(4), 1057-1065 (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.

#### WARRANTY AND LIMITATION OF REMEDY

Buyer agrees to purchase the material subject to Cayman's Terms and Conditions. Complete Terms and Conditions including Warranty and Limitation of Liability information can be found on our website.

Copyright Cayman Chemical Company, 11/04/2019

#### 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