

CAY10727

## Chemical Properties

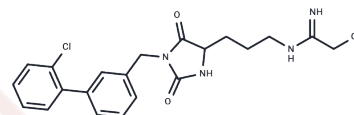
CAS No. : 1671088-84-8

Formula: C<sub>21</sub>H<sub>22</sub>Cl<sub>2</sub>N<sub>4</sub>O<sub>2</sub>

Molecular Weight: 433.33

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Actual storage temperature shall be subject to the COA.



## Biological Description

Description	CAY10727 is an inhibitor of protein arginine deiminase 3 (PAD3; $k_{inact}/K_i = 15,600 \text{ M}^{-1}\text{min}^{-1}$ ). It is selective for PAD3 over PAD1, -2, and -4 ( $k_{inact}/K_i = 360, 1,110, \text{ and } 1,460 \text{ M}^{-1}\text{min}^{-1}$ , respectively).
Targets(IC <sub>50</sub> )	Others,PAD

## Solubility Information

Solubility	DMF: 30 mg/mL (69.23 mM),Sonication is recommended. DMSO: 30 mg/mL (69.23 mM),Sonication is recommended. DMSO:PBS (pH 7.2) (1:1): 0.5 mg/mL (1.15 mM),Sonication is recommended. Ethanol: 10 mg/mL (23.08 mM),Sonication is recommended. ( $< 1 \text{ mg/ml}$ refers to the product slightly soluble or insoluble)
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## Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.3077 mL	11.5386 mL	23.0771 mL
5 mM	0.4615 mL	2.3077 mL	4.6154 mL
10 mM	0.2308 mL	1.1539 mL	2.3077 mL
50 mM	0.0462 mL	0.2308 mL	0.4615 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

## Reference

Jamali, H., Khan, H.A., Stringer, J.R., et al. Identification of multiple structurally distinct, nonpeptidic small molecule inhibitors of protein arginine deiminase 3 using a substrate-based fragment method. *J. Am. Chem. Soc.* 137(10) 3616-3621(2015)

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