

Product Data Sheet

Product Name: CAY10727

Cat. No.: GC47050

Chemical Properties

Cas. No. 1671088-84-8

SMILES C1C=CC=CC=C1C2=CC=CC(CN3C(NC(CCCNC(CCl)=N)C3=O)=O)=C2

Formula C₂₁H₂₂Cl₂N₄O₂

M.Wt 433.3

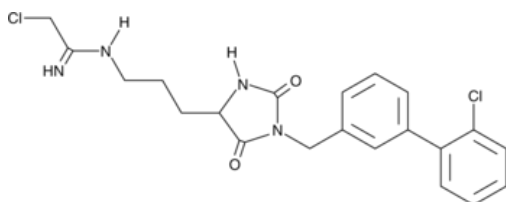
Solubility DMF: 30 mg/ml, DMSO: 30 mg/ml, DMSO:PBS (pH 7.2) (1:1): 0.5 mg/ml, Ethanol: 10 mg/ml

Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure



Background

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

1. 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)

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com

Address: 10292 Central Ave. #205, Montclair, CA, USA