

CAY10761

Chemical Properties

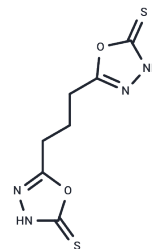
CAS No. : 333409-31-7

Formula: C₇H₈N₄O₂S₂

Molecular Weight: 244.29

Appearance:

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



Biological Description

| | |
|----------------------------|---|
| Description | CAY10761 is an inhibitor of ectonucleotide pyrophosphatase/phosphodiesterase 1 (ENPP1; IC ₅₀ s = 467 and 429 μM for the human and snake venom enzymes, respectively). ^{1,2} It also inhibits mushroom tyrosinase (K _i = 1.9 μM) and urease from jack bean, <i>P. mirabilis</i> , and <i>B. pasteurii</i> (IC ₅₀ s = 0.093, <0.125, and 0.089 mM, respectively, at pH 8.2). ^{3,4} |
| Targets(IC ₅₀) | Others |

Solubility Information

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|------------|--|
| Solubility | DMF: 30 mg/mL (122.8 mM), Sonication is recommended. DMSO: 30 mg/mL (122.8 mM), Sonication is recommended. DMSO:PBS (pH 7.2) (1:4): 0.2 mg/mL (0.82 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble) |
|------------|--|

Preparing Stock Solutions

| | 1mg | 5mg | 10mg |
|-------|-----------|------------|-----------|
| 1 mM | 4.0935 mL | 20.4675 mL | 40.935 mL |
| 5 mM | 0.8187 mL | 4.0935 mL | 8.187 mL |
| 10 mM | 0.4093 mL | 2.0467 mL | 4.0935 mL |
| 50 mM | 0.0819 mL | 0.4093 mL | 0.8187 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.

Reference

- Khan, K.M., Fatima, N., Rasheed, M., et al. 1,3,4-Oxadiazole-2(3H)-thione and its analogues: A new class of non-competitive nucleotide pyrophosphatases/phosphodiesterases 1 inhibitors. *Bioorg. Med. Chem.* 17(22), 7816-7822 (2009).
- Onyedibe, K.I., Wang, M., and Sintim, H.O. ENPP1, an old enzyme with new functions, and small molecule inhibitors - A STING in the tale of ENPP1. *Molecules* 24(22), E4192 (2019).
- Ghani, U., and Ullah, N. New potent inhibitors of tyrosinase: Novel clues to binding of 1,3,4-thiadiazole-2(3H)-thiones, 1,3,4-oxadiazole-2(3H)-thiones, 4-amino-1,2,4-triazole-5(4H)-thiones, and substituted hydrazides to the dicopper active site. *Bioorg. Med. Chem.* 18(11), 4042-4048 (2010).
- Amtul, Z., Rasheed, M., Choudhary, M.I., et al. Kinetics of novel competitive inhibitors of urease enzymes by a focused library of oxadiazoles/thiadiazoles and triazoles. *Biochem. Biophys. Res. Commun.* 319(3), 1053-1063 (2004).

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