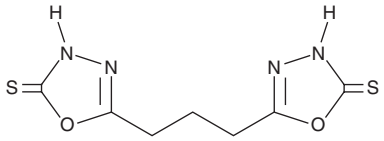
PRODUCT INFORMATION

CAY10761

Item No. 29865

CAS Registry No.:	333409-31-7
Formal Name:	5,5′-(1,3-propanediyl)*bis*-1,3,4-oxadiazole-2(3H)-thione
MF:	$C_7H_8N_4O_2S_2$
FW:	244.3
Purity:	≥98%
UV/Vis.:	λ_{max}: 266 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

CAY10761 is supplied as a crystalline solid. A stock solution may be made by dissolving the CAY10761 in the solvent of choice, which should be purged with an inert gas. CAY10761 is soluble in organic solvents such as DMSO and dimethyl formamide. The solubility of CAY10761 in these solvents is approximately 30 mg/ml.

CAY10761 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, CAY10761 should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. CAY10761 has a solubility of approximately 0.2 mg/ml in a 1:4 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

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, *P. mirabilis*, and *B. pasteurii* (IC_{50}s = 0.093, <0.125, and 0.089 mM, respectively, at pH 8.2).[3,4]

References

1. Khan, K.M., Fatima, N., Rasheed, M., *et al.* 1,3,4-Oxadiazole-2(3*H*)-thione and its analogues: A new class of non-competitive nucleotide pyrophosphatases/phosphodiesterases 1 inhibitors. *Bioorg. Med. Chem.* **17(22)**, 7816-7822 (2009).
2. 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).
3. Ghani, U., and Ullah, N. New potent inhibitors of tyrosinase: Novel clues to binding of 1,3,4-thiadiazole-2(3*H*)-thiones, 1,3,4-oxadiazole-2(3*H*)-thiones, 4-amino-1,2,4-triazole-5(4*H*)-thiones, and substituted hydrazides to the dicopper active site. *Bioorg. Med. Chem.* **18(11)**, 4042-4048 (2010).
4. 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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