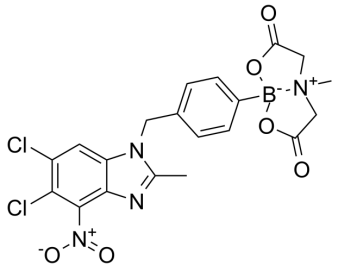
TH1217

Cat. No.:	HY-135909
CAS No.:	1862212-48-3
Molecular Formula:	$C_{20}H_{17}BCl_2N_4O_6$
Molecular Weight:	491.09
Target:	SARS-CoV
Pathway:	Anti-infection
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 125 mg/mL (254.54 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.0363 mL	10.1814 mL	20.3629 mL
	5 mM	0.4073 mL	2.0363 mL	4.0726 mL
	10 mM	0.2036 mL	1.0181 mL	2.0363 mL

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description

TH1217 (ZINC1775962367) is a potent and selective dCTPase pyrophosphatase 1 (dCTPase) inhibitor, with an IC_{50} of 47 nM. TH1217 enhances the cytotoxic effect of cytidine analogues in leukemia cells. TH1217 also could modulate SARS-Cov-2 interactors, so it shows activity of against COVID-19[1][2].

IC_{50} & Target

IC50: 47 nM (dCTPase)[1]

In Vitro

TH1217 (compound 30) inhibits dCTPase and enhances aqueous solubility (>100 μM) and improves plasma stability in vitro(t_{4h}=86%)[1].

TH1217 presents suitable mouse microsomal half-lives (109 minutes)[1].

TH1217 displays well cell permeability (8.66×10^{-6}/1.30×10^{-3} cm/s) and CYP inhibition[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Nucleic Acids Res. 2021 Jan 8;49(D1):D1113-D1121.

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REFERENCES

[1]. Llona-Minguez S, et, al. Discovery of the First Potent and Selective Inhibitors of Human dCTP Pyrophosphatase 1. Med Chem. 2016 Feb 11; 59(3): 1140-1148.

[2]. Gordon DE, et, al. A SARS-CoV-2-Human Protein-Protein Interaction Map Reveals Drug Targets and Potential Drug-Repurposing. bioRxiv. 2020 Mar 22; 2020.03.22.002386.

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