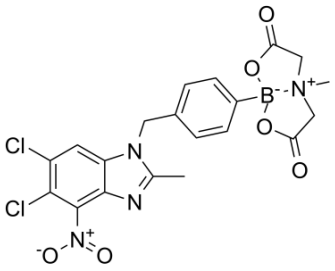
TH1217

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:	Please store the product under the recommended conditions in the Certificate of Analysis.



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.

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.

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

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