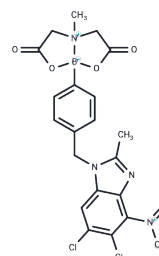


TH1217

Chemical Properties

CAS No. : 1862212-48-3
 Formula: C₂₀H₁₇Cl₂N₄O₆
 Molecular Weight: 491.09
 Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
 Actual storage temperature shall be subject to the COA.



Biological Description

Description	TH1217, a potent and selective inhibitor of dCTPase pyrophosphatase 1 (dCTPase), demonstrates an IC ₅₀ value of 47 nM. It amplifies the cytotoxic impact of cytidine analogues on leukemia cells and exhibits potential against COVID-19 by modulating SARS-CoV-2 interactors.
Targets(IC ₅₀)	Others,SARS-CoV
In vitro	TH1217 (compound 30) inhibits dCTPase, enhances aqueous solubility (>100 μM), and improves plasma stability in vitro (t _{4h} =86%), with suitable mouse microsomal half-lives (109 minutes). TH1217 displays good cell permeability (8.66×10 ⁻⁶ /1.30×10 ⁻³ cm/s) and CYP inhibition[1].

Solubility Information

Solubility	DMSO: 117 mg/mL (238.25 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
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Preparing Stock Solutions

	1mg	5mg	10mg
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
50 mM	0.0407 mL	0.2036 mL	0.4073 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.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Llona-Minguez et al (2016) Discovery of the first potent and selective inhibitors of human dCTP pyrophosphatase 1. J.Med.Chem. 59 1140

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.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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