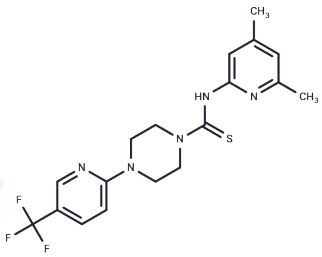
Data Sheet (Cat.No.T16277)

TargetMol

NCT-502

Chemical Properties



CAS No. : 1542213-00-2

Formula: C18H20F3N5S

Molecular Weight: 395.45

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	NCT-502 (N-(4,6-dimethylpyridin-2-yl)-4-[5-(trifluoromethyl)pyridin-2-yl]piperazine-1-carbothioamide) is a human phosphoglycerate dehydrogenase inhibitor, cytotoxic to PHGDH-dependent cancer cells. It decreases glucose-derived serine production and it has an IC50 of 3.7 μM against PHGDH.
Targets(IC50)	Dehydrogenase
In vitro	NCT-502 is cytotoxic to MDA-MB-468 (EC50: 15.2 μM)[1].

Solubility Information

Solubility	H2O: < 0.1 mg/mL (insoluble) DMSO: 55 mg/mL (139.08 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (5.06 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.5288 mL	12.6438 mL	25.2876 mL
5 mM	0.5058 mL	2.5288 mL	5.0575 mL
10 mM	0.2529 mL	1.2644 mL	2.5288 mL
50 mM	0.0506 mL	0.2529 mL	0.5058 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

Rohde JM, et al. Discovery and optimization of piperazine-1-thiourea-based human phosphoglycerate dehydrogenase inhibitors. Bioorg Med Chem. 2018 May 1;26(8):1727-1739.