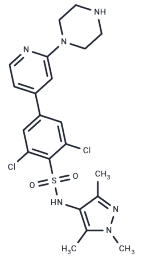
Data Sheet (Cat.No.T27135)

TargetMol

DDD85646

Chemical Properties



CAS No. : 1215010-55-1

Formula: C21H24Cl2N6O2S

Molecular Weight: 495.43

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	DDD85646 is an inhibitor of T. brucei N-myristoyltransferase with a Ki of 1.44 nM, an IC50 of 2 nM and an EC50 of 2 nM. The IC50 of hNMT is 4 nM.
Targets(IC50)	Parasite,DNA/RNA Synthesis

Solubility Information

Solubility	DMSO: 95 mg/mL (191.75 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: 3.3 mg/mL (6.66 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	2.0184 mL	10.0922 mL	20.1845 mL
5 mM	0.4037 mL	2.0184 mL	4.0369 mL
10 mM	0.2018 mL	1.0092 mL	2.0184 mL
50 mM	0.0404 mL	0.2018 mL	0.4037 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

Bayliss T, Robinson DA, Smith VC, Brand S, McElroy SP, Torrie LS, Mpamhanga C, Norval S, Stojanovski L, Brenk R, Frearson JA, Read KD, Gilbert IH, Wyatt PG. Design and Synthesis of Brain Penetrant Trypanocidal N-Myristoyltransferase Inhibitors. J Med Chem. 2017 Nov 10. doi: 10.1021/acs.jmedchem.7b01255. [Epub ahead of print] PubMed PMID: 29125744.

Roberts AJ, Fairlamb AH. The N-myristoylome of Trypanosoma cruzi. Sci Rep. 2016 Aug 5;6:31078. doi: 10.1038/srep31078. PubMed PMID: 27492267; PubMed Central PMCID: PMC4974623.

Robinson DA, Wyatt PG. Identification and structure solution of fragment hits against kinetoplastid N-myristoyltransferase. Acta Crystallogr F Struct Biol Commun. 2015 May;71(Pt 5):586-93. doi: 10.1107/S2053230X15003040. Epub 2015 Apr 21. PubMed PMID: 25945713; PubMed Central PMCID: PMC4427169.

Fang W, Robinson DA, Raimi OG, Blair DE, Harrison JR, Lockhart DE, Torrie LS, Ruda GF, Wyatt PG, Gilbert IH, van Aalten DM. N-myristoyltransferase is a cell wall target in Aspergillus fumigatus. ACS Chem Biol. 2015 Jun 19;10(6):1425-34. doi: 10.1021/cb5008647. Epub 2015 Feb 27. PubMed PMID: 25706802; PubMed Central PMCID: PMC4477619.